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(54) Title: **NUCLEAR RECEPTOR STRUCTURE**

(57) Abstract: The present invention is in the fields of biotechnology, protein purification and crystallization, x-ray diffraction analysis, three-dimensional computer molecular modeling and rational drug design. The invention is directed to the glucocorticoid receptor and ligands for this receptor, and in particular to crystalline glucocorticoid receptor (GR) and to methods of identifying ligands utilizing GR, as well as to compounds, compositions and methods for selecting, making, and using therapeutic or diagnostic agents having GR modulating or binding activity.

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### FIELD OF THE INVENTION

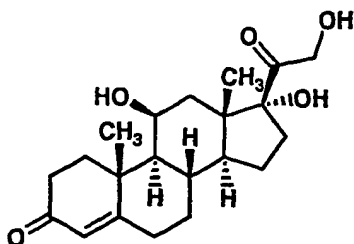
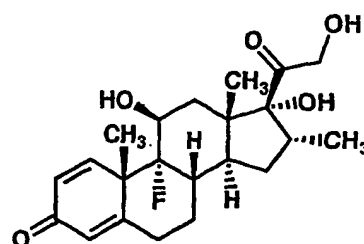
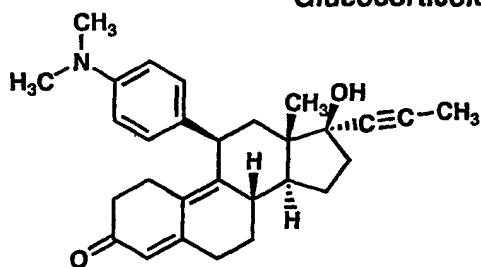
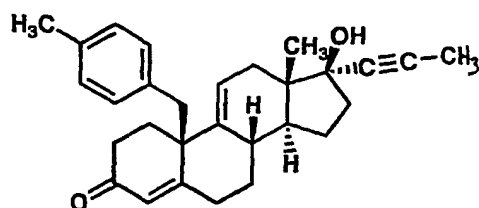
The present invention is in the fields of biotechnology, protein purification and crystallization, x-ray diffraction analysis, three-dimensional computer molecular modeling and rational drug design. The invention is directed to the glucocorticoid receptor and ligands for this receptor, and in particular to crystalline glucocorticoid receptor (GR) and to methods of identifying ligands utilizing GR, as well as to compounds, compositions and methods for selecting, making, and using therapeutic or diagnostic agents having GR modulating or binding activity.

### BACKGROUND OF THE INVENTION

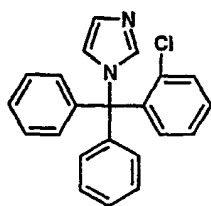
The three-dimensional structures of the ligand binding domains of the estrogen (ER) (Brzozowski, A.M., *et al.*, *M. Nature* **1997**, 389, 753-758), progesterone (PR) (Williams, S.P.; Sigler, P.B. *Nature* **1998**, 393, 392-396), and of the androgen (AR) (Matias, P.M.; *et al.*, *J Biol Chem* **2000**, 275, 26164-26171) receptors have been determined. Knowledge of the three-dimensional structure has enabled a better understanding of the modes of ligand binding to steroidal nuclear receptors and the determination of the optimum conformation of ligand to bind to these receptors. This understanding will provide a pharmacophore model usable in the design of ligands, such as drugs, to bind to the glucocorticoid receptor. It is generally believed in the art that the AR, ER, and PR structures also provide a guide to the design of GR ligands.

Glucocorticoid steroid hormone and thus the glucocorticoid receptor (GR) is a member of the steroid hormone nuclear receptor family. Its primary natural ligand in human is cortisol. Cortisol and a large number of synthetic steroids such as dexamethasone have an agonist mechanism of action (they up-regulate genes downstream from glucocorticoid response elements (GREs)). A number of synthetic glucocorticoid antagonists have also been described in the literature and these include RU-38,486 and RU-43,044.

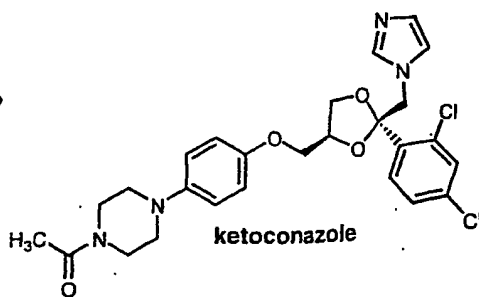
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**Glucocorticoid Agonists****cortisol****dexamethasone****Glucocorticoid Antagonists****RU-38,486****RU-43,044**

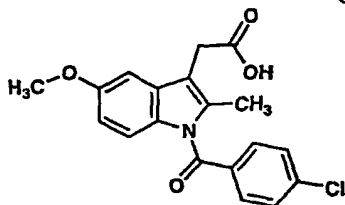
However, it is known that a large number of structurally diverse non-steroidal compounds such as clotrimazole, ketoconazole (WO-09932101; J. Clin. Invest. 1983, 72, 404-408.), indomethacin (Biochem. Pharmacol. 1978, 27, 1187-91.), collismycin (J. Antibiot. 1994, 47, 1072-4.), N-(2,3,3-triphenylpropyl)-2-thiopheneacetamide (WO-09933786), 4-aminotriphenyl-methanes (WO-00006137), benzopyranoquinolines (WO-09941256), benzo[3,4-f]quinolines (WO-09941257), 2-hydroxy-4-(2-hydroxyphenyl)alkylamino-substituted heterocycles (WO-00032584), (4bR,7S,8aS)-rel-4b,5,6,7,8,8a,9,10-octahydro-7-hydroxy-4b-(phenylmethyl)-7-(1-propynyl)-2-phenanthrenecarbonitrile (WO-0066522), and (3,5-dibromo-4-[5-isopropyl-4-methoxy-2-(3-methylbenzoyl)-phenoxy]phenyl)acetic acid (WO-09963976) also bind to the glucocorticoid receptor.



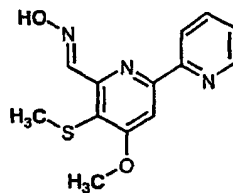
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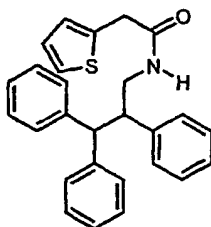
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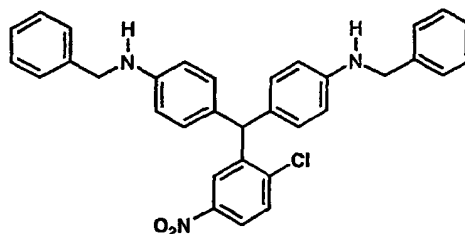
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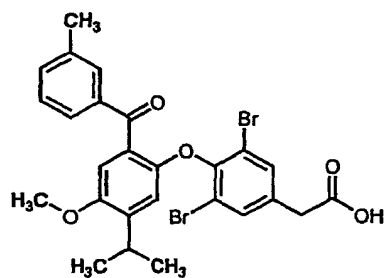
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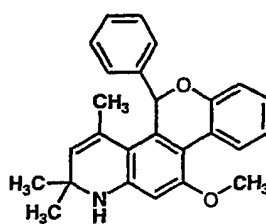
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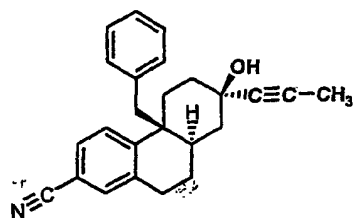
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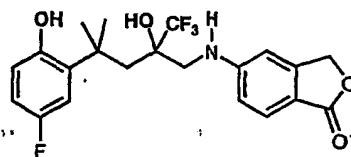
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WO-09941257



WO-0066522



WO-00032584

It has been proposed that the receptor possesses a multi-functional modular structure potentially having discrete domains for DNA binding, ligand binding, and transactivation. The ligand binding domain (LBD) has been designated domain E and is the largest domain of the glucocorticoid receptor. The ligand binding domain includes a ligand recognition site and regions for receptor dimerization, interaction with heat shock proteins, nuclear localization and ligand dependent transactivation.

A review of the structure and functioning of the glucocorticoid receptor is provided in an article by Gustafsson, J.Å. et al., *Prog Clin Biol Res* 1990, 322, 65-80.

It is known that compounds which bind to the glucocorticoid receptor are potentially useful in the treatment a wide range of disease states. These include glucocorticoid agonists for treatment of disease linked to glucocorticoid deficiency (e.g., Addison's Disease) and for treatment of autoimmune and inflammatory diseases and glucocorticoid antagonists for treatment disease linked to glucocorticoid excess such as Cushing Syndrome and type-II diabetes. Furthermore, it is known that certain ligands such as RU-24,858, ZK-079,642, and medroprogesterone acetate display a dissociated mechanism of action (trans-repress AP-1 and/or NF- $\kappa$ B without transactivating through binding to classical glucocorticoid response elements). It is further known that a number of structurally diverse classes of steroidal and non-steroidal ligands are usable as agonists or antagonists to the glucocorticoid receptor, and that it is possible to modify their binding mechanics, for example the binding affinity, by changing the substituent groups at various positions on the molecule. Therefore, it would be desirable to be able to design ligands which are recognizable by and able to bind to the glucocorticoid receptor. Additionally, it would be desirable to know the three dimensional structure of the glucocorticoid receptor. Such knowledge would be useful for the design of compounds intended to bind to the glucocorticoid receptor. Difficulties in obtaining GR crystals resulted in a GR model being developed on the basis of thyroid hormone, estrogen and progesterone receptors (WO 00/52050). However, the present inventors now have been able to produce a glucocorticoid receptor crystal and to determine from that the three dimensional structure of the glucocorticoid receptor. Unexpectedly, the thus determined GR structure reveals that the AR, ER, and PR structures do not provide a

good model for binding of ligands to GR.

### SUMMARY OF THE INVENTION

We have succeeded in crystallizing GR and determining its crystallographic co-ordinates. Therefore, in a first aspect the present invention provides a glucocorticoid receptor ligand binding domain crystal.

In another aspect of the invention, methods for designing ligands which will bind to GR are provided. Such methods use three-dimensional models based on the crystals of the glucocorticoid receptor. Generally, such methods comprise, determining compounds which are likely to bind to the receptor based on their three dimensional shape in particular the ligand binding domain of the GR. Preferably, those compounds have a structure which is complementary to that of the GR. Such methods comprise the steps of determining which amino acid or amino acids of the ligand binding domain of the GR interacts with the binding ligand, and selecting compounds or modifying existing compounds, to improve the interaction. Preferably, improvements in the interaction are manifested as increases in the binding affinity but may also include increases receptor selectivity and/or modulation of efficacy.

Preferably, the ligands bind to the internal GR binding cavity with a high binding affinity, for example within the range of 0.01–100 nM.

The ligands may bind tightly to the GR yet not up-regulate gene expression thereby inhibiting the action of cortisol and cortisol mimetics. Thus, the invention also provides a method of inhibiting the activity of cortisol or cortisol mimetics by providing ligands which bind to GR with a high affinity, blocking the activity of glucocorticoids. Alternatively, binding of the ligand to the GR may cause conformational changes to the GR inhibiting further binding thereto. The invention further provides a method of inhibiting cortisol activity in an animal, the method comprising administering to the animal a ligand which binds to at least the LBD, of the GR with high affinity and blocks binding of further ligands to at least the LBD of the GR. Such ligands are useful in, for example, the treatment of glucocorticoid receptor mediated diseases in humans. Preferably the ligands are identified by the

method of designing ligands according to the invention.

Protein crystallography is not routine. For example, during the process of finding a crystallisable species, a number of GR constructs were designed. The starting point was the PR crystal and the visible part of PR in electron density. Sequence alignment showed the corresponding GR position. Quite unexpectedly the constructs most similar to PR did not produce GR protein suitable for crystallisation. Over 15 additional residues were necessary for the production of GR that could be homogeneously crystallised.

#### DETAILED DESCRIPTION OF THE INVENTION

One aspect of the invention provides a crystal comprising at least 150 amino acid residues of the GR ligand binding domain. Preferably, the said crystal comprises at least 175, or at least 200, or at least 240 amino acid residues of GR. More preferably, said crystal contains at least 250 amino acid residues of GR. Most preferably, the said crystal comprises the entire GR amino acid sequence.

Preferably the crystal comprises the amino acid sequence shown as Leu-532 to Leu-732, especially Leu-532 to Met-745, most preferably Leu-532 to Gln-776, of a GR ligand binding domain as shown in Figure 7 or an amino acid sequence having at least 95%, especially above 97, 98 or 99% identity to the sequence. This numbering is based on the full GR sequence.

Most preferably the crystal comprises Leu-532 to Met-745, especially Leu-532 to Gln-776.

The sequences of GR1, GR2 and GR3 are shown as Seq. ID1, 2 and 3 respectively. The amino acid numbering consequently changes to reflect the sequence listing numbering. Most preferably the crystals have one or more of the properties shown in Table 1.

Preferably the amino acid sequence of the crystal comprises Leu-35 to Leu-235, especially Leu-35 to Met-248, more preferably Leu 35 to Gln-279 of GR1 (shown as Seq. ID. No. 1). Preferably the crystal comprises the entire sequence of GR1.

The amino acid sequence of the crystal may comprise Leu-14 to Leu-214, most preferably the entire sequence of GR2 (shown as Seq ID No. 2).

Alternatively the amino acid sequence of the crystal may comprise Leu-35 to Leu-235, preferably Leu-35 to Met-248, more preferably Leu-35 to Glu-279, especially the entire sequence shown for GR3 (shown as Seq ID No. 3).

Isolated proteins consisting of the amino acid sequences listed for the crystals are also provided by the invention. The isolated proteins may be used to produce the crystals.

The proposed structural identity of parts of the GR ligand binding domain is shown below, based on the amino acid numbering of the full GR sequence in comparison with the equivalent structural elements for Estrogen Receptor Ligand binding domains.

GR#	ER#	GR residues
helix-1	(H2)	Leu-532 to Ile-539
helix-2	(H3)	Thr-556 to Lys-579
helix-3	(H5)	Leu-589 /Asp-591 to Gln-615/Ser-616
sheet-1	(S1)	Leu-621 to Cys-622/Ala-624
sheet-2	(S2)	Leu-627/Ile-628 to Ile-629
helix-4	(H7)	Met-639/Tyr-640/Cys-643 to Arg-655
helix-5	(H8)	Tyr-660 to Leu-671
sheet-3	(NA)	Ser-674 to Pro-676
sheet -4	(NA)	Ile-679 to Lys-771
helix-6	(H9)	Gln-583 to Val-702/Lys-703/Arg-704
helix-7	(H10-11)	Gln-710/Asn-711 to Leu-732/Cys-736
helix-8	(NA)	Phe-740 to Met-745
helix-9	(H12)	Phe-749 to Ile-757

NA = Not applicable (corresponding secondary structural element does not exist in ER).

An embodiment of this aspect of the invention provides a crystal produced using a sequence including helix 9 of GR. Preferably this is between Phe-749 to Ile-757, especially Leu-753 to Ile-757.

The crystals according to the invention may be usable in X-ray crystallography.

In another embodiment of the present invention there is provided a GR crystal as described above also including a ligand bound to GR or a portion thereof. Said ligand may be selected from RU-486 [(11 $\beta$ ,17 $\beta$ )-11-[4-(dimethylamino)phenyl]-17-hydroxy-17-(1-propynyl)-estra-4,9-dien-3-one, CAS registry number 84371-65-3], cortisol, dexamethasone or any other ligand that binds with high affinity (<1.0 nM) to the internal GR binding cavity. The dexamethasone may be used with a coactivator ligand such as T1F2 NR-box 3.

In another embodiment of the present invention there is provided a crystal of GR LDB belonging to the space group  $P2_12_12_1$  and having the unit cell dimensions  $a = 67.33$  Å,  $b = 87.42$  Å,  $c = 93.11$  Å,  $\alpha = \beta = \gamma = 90^\circ$ .

In another embodiment of the present invention there is provided a crystal of GR LDB belonging to the space group  $P6_3$  and having the unit cell dimensions  $a = 132.09$  Å,  $b = 132.09$  Å,  $c = 53.048$  Å,  $\alpha = \beta = 90^\circ$ ,  $\gamma = 120^\circ$ .

In another embodiment of the present invention there is provided a crystal of GR LDB belonging to the space group  $P2_12_12_1$  and having the unit cell dimensions  $a = 74.5$  Å,  $b = 109.7$  Å,  $c = 39.1$  Å,  $\alpha = \beta = \gamma = 90^\circ$ .

A preferred crystal belongs to the  $p3_1$  space group with a pair of dimers in the

asymmetric unit, and having cell dimensions  $a=b=127.4$ ,  $c=91.8$ ,  $\alpha=\beta=90^\circ$ ,  $\gamma=120^\circ$ .

The crystals according to the invention may have a resolution as determined by X-ray crystallography of less than  $3.6\text{\AA}$ , preferably less than  $2.9\text{\AA}$ .

In another aspect of the present invention, there is provided a machine-readable data storage medium, comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a crystal structure as described above or a homologue of said crystal structure. Homologues include crystals with the same space group, but with another ligand, crystals with the same space group and substantially the same dimensions, and crystals using GR from other species such as rat.

In yet another aspect of the present invention, there is provided a method for designing a potential glucocorticoid receptor ligand for the treatment of diseases modulated by the glucocorticoid, the method comprising the steps of:

- a) employing computational means to perform a fitting operation between the chemical entity and a binding site of GR receptors identified from a crystal of the invention, machine-readable storage medium as described above or a 3D representation obtained from the storage medium;
- b) analyzing the results of the fitting operation to predict the association between the potential chemical entity and the binding site;
- c) synthesizing the potential glucocorticoid receptor ligand based on the crystal structure of the glucocorticoid receptor;
- d) assaying the glucocorticoid receptor ligand for glucocorticoid receptor binding, response in a glucocorticoid reporter cell line, measuring in vivo effects including but not limited to hepatic glucose production, marker proteins such as transamino transferase, corticotropin-releasing hormone,

or anti-inflammatory response which indicates that the compound may be used for treatment of diseases modulated by the glucocorticoid receptor.

The binding pocket residues have preferably been identified.

In yet another aspect of the present invention, there is provided a method of designing a ligand which will bind to GR comprising comparing the shape of a compound with the shape of the ligand binding domain of GR as obtained from a crystal according to the invention, and determining which amino acid or amino acids of the ligand binding domain interact with said compound.

Ligands identified by the methods of designing ligands are also included in the scope of the invention. Preferably, there are agonists or antagonists of GR.

Preferably, the ligands interact with Arg611 and Gln642 which have been shown to be important determining the GR specificity of ligands.

In yet another aspect of the present invention, there is provided a crystallized molecule or molecular complex comprising a binding pocket defined by the structure coordinates of human GR ligand binding domain amino acid residues MET560, LEU563, ASN564, LEU566, GLY567, GLY568, GLN570, TRP600, MET601, MET604, ALA605, LEU608, PHE623, MET646, LEU732, CYS736, ALA748 or a homologue of said molecule or molecular complex wherein said homologue has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

A further aspect of the invention provides crystalisable compositions comprising at least 150 amino acid residues of the GR ligand binding domain.

## STRUCTURE BASED DESIGN OF GR LIGANDS

The present invention elucidates the structure of the ligand binding cavity of GR.

Knowledge of the structure of this cavity has utility in the design of structurally novel GR ligands and in the design of non-obvious analogs of known GR ligands with improved properties. These enhanced properties include one or more of the following: (1) higher affinity, (2) improved selectivity for GR vs. closely related nuclear hormone receptors such as MR, and/or (3) a designed degree of efficacy (agonism vs. partial agonism vs. antagonism). Without knowledge of the GR structure, modifications to produce ligands with enhanced properties and a reasonable likelihood of success would not be available to those skilled in the art. The GR structure also has utility in the discovery of new, structurally novel classes of GR ligands. Electronic screening of large, structurally diverse compound libraries such as the Available Chemical Directory (ACD) will identify new structural classes of GR ligands which will bind to the 3-dimensional structure of the glucocorticoid receptor. Additionally the GR structure allows for "reverse-engineering" or "*de novo* design" of compounds to bind to GR.

#### **(1) Enhanced Affinity**

The present invention has revealed the presence of glucocorticoid receptor beta defined  $\beta$ - and  $\alpha$ -face cavities centered respectively above and below the B- and C-rings of cortisol.

The present invention provides new ligands which exploit this discovery by filling the  $\alpha$ - and  $\beta$ -face cavities.

Preferably, the ligand fills at least one of the  $\alpha$ - and  $\beta$ -face cavities so as to displace water from the cavity or cavities.

The ligands produced in accordance with the invention bind more effectively to the GR than cortisol. The ligand may bind with twice the binding affinity of cortisol, preferably three times the affinity, and most preferably ten or more times the affinity.

Modifications to the steroid nucleus may be made at the positions marked in R in Figure 1 ( $\alpha$ -substitution at the 7-, 9-, 12-, 14-, 16-, and 17-positions;  $\beta$ -substitution at

the 8-, 11-, 15-, and 18-positions). Preferably, those substituents are hydrophobic substituents, e.g., methyl, ethyl, iso-propyl, fluorine, chlorine, bromine, or iodine.

Preferably, the ligand produced in accordance with the invention fills at least one of the  $\alpha$ - and  $\beta$ -cavities of the GR without perturbing the remainder of the GR structure.

## **(2) Improved Selectivity**

The glucocorticoid receptor is closely related to the progesterone and mineralocorticoid receptors. The glucocorticoid, mineralocorticoid, and progesterone receptors differ significantly in their primary sequence and slightly in their tertiary structure. As a consequence of these receptor differences, ligands may bind with different affinity to these three receptors.

Furthermore, a detailed understanding of the different receptors enables the different behavior of a compound in different tissues to be understood, for example the glucocorticoid behavior of dissociated glucocorticoids or selective glucocorticoid receptor modulators (SGRMs) on the tissue in which it is active.

The present invention provides new ligands which exploit these differences by positioning ligand substituents in close proximity to one or more amino acid residue that differ between GR and PR, MR, or AR.

The ligands produced in accordance with the invention bind more effectively to the glucocorticoid receptor than to the mineralocorticoid, progesterone, or androgen receptor. The selectivity of the binding to the glucocorticoid receptor may be ten-fold, more preferably one hundred-fold, and most preferably greater than one thousand-fold.

This invention also provides a means of enhancing the selectivity of other classes of non-steroidal GR ligands.

## **(3) Modulation of Efficacy**

This invention provides an understanding of the differences between glucocorticoid

and antiglucocorticoid binding and therefore a means to design GR ligands with the desired degree of efficacy. An examination of the differences between the GR/RU-486 and PR/progesterone complexes reveals a large movement in Helix-9 (Fig 4.). H9 adopts an "agonistic" conformation defined by the structure of the PR/progesterone complex and an "antagonistic" conformation defined by the structure of the GR/ RU-486 complex. These two conformations are in thermodynamic equilibrium. When the GR is complexed with a full agonist, such as cortisol, the equilibrium lies far in the direction of the "agonistic" conformation. In contrast, while when complexed with an antagonist, the equilibrium is pushed in the direction of the "antagonistic" conformation. In the case of RU-486, the 11-beta aryl substituent sterically collides with H9 in its agonistic conformation, thereby driving the equilibrium strongly in the antagonistic direction. By introduction of progressively shorter side chains at 11-beta position of RU-486, the equilibrium will be gradually shifted back towards the agonist conformation. Thus, this invention provides a means of developing ligands with the desired degree of efficacy (agonist, partial agonist, or antagonist).

In particular, the importance of H9 has been determined as playing a central role in determining the efficacy (agonism vs. antagonism) of a ligand. Thus, ligands which are able to bind to and/or alter the conformation of H9 are of particular importance when designing a ligand or assessing the binding of a ligand, for the glucocorticoid receptor.

Additionally, it has been found that at least the majority of such receptor proteins when activated by binding to an agonist ligand are in the form a dimer (Khorasanizadeh S, Rastinejad F. "Nuclear-receptor interactions on DNA-response elements." Trends Biochem Sci. 2001 Jun;26(6):384-90.). Such dimerization leads to a potential route for disruption. Disruptions of this type can be used to predict antagonism or to produce antagonists. Disruptions may take the form of ligand binding which alters the conformation of the helices that comprise the dimerization interface or direct binding to the dimerization interface which then inhibits dimerization.

Further, the orientation of the ligand may be keyed to the receptor, in the dimeric or monomeric form. Furthermore, using the crystals of the present invention, the influence of ligand binding to the LDB on the receptor conformation can now be shown to have influences on the behavior of the receptor since it may disrupt the binding of co-activator, co-repressor, or heat-shock proteins. Previously, such predictions could not be made.

In the GR crystal structures identified the side chains involved in building up the ligand binding cavity are revealed. The ligand is well defined in the electron density map. Superposition of the ligand binding sites of the homologous agonist structures GR4 (dexamethasone), PR (PDB # 1A28, progesterone) and AR (PDB # 1I37, dihydrotestosterone). The A-ring side of the steroid hormone is situated in the most conserved protein side chain environment, with Phe623, Arg611, and Gln570, respectively, at identical positions (taking the error of the models in consideration). All these ligands are also very similar in their A and B-rings. On the D-ring side, on the other hand, unique features exist between different steroid ligands consistent with larger differences between corresponding cognate receptors in the D-ring-harboring part of the ligand-binding pocket. The largest variation in structure between the three receptor LBD's is seen for Gln642 (Leu797 in PR, Gln783 in AR). In GR, Gln642 makes a hydrogen bond to the 17 $\alpha$ -hydroxy group. The position of the side-chains of the three other residues in GR-LBD that bind to the C/D-ring of the steroid (Asn564, 11 $\beta$ -hydroxy; Cys736, 20-keto; Thr739, 21-hydroxy) are relatively well conserved between the three structures. Thus, Gln642 appears to play a unique role in steroid recognition.

The binding of ligands is expected to alter GR activity. For example, the antihormone RU-486 (mifepristone) is an effective antiprogesterin and antiglucocorticoid that has shown clinical efficacy in both functions. It is also a weak antiandrogen. The function of the antagonistic action of RU-486 has been shown to be an active process and not just the blocking of agonist binding. Following the binding of RU-486, GR binds more tightly to specific DNA sequences with a slower dissociation rate. The antagonist ZK98299 appears to induce a differential PR conformation that affects the interaction with DNA. Thus, there is an interdomain functional interaction that is

dependent on the ligand bound. Further evidence of this has been found with regard to ligand-dependent phosphorylation of GR. Whereas both dexamethasone and RU-486 induce phosphorylation of Ser203, dexamethasone but not RU-486 induces phosphorylation of Ser211. This differential phosphorylation pattern was related to the intracellular location of the subspecies of GR. Binding of RU-486 blocks the binding of coactivators at the AF-2 site while simultaneously actively recruiting the binding of corepressor NCoR or SMRT. This function is again dependent on the N-terminal domain of GR although the corepressor interaction site is complex and involves sequences within the ligand-binding domain as well. In various model systems, RU-486 can act as an agonist in the absence of corepressor, acting through the N-terminal AF-1 site. The agonist function of RU-486 can also be shown for specific glucocorticoid-induced phenotypes such as the induction of p27<sup>Kip1</sup>, part of the cytostatic action of glucocorticoids in osteosarcoma cells. A similar active antagonistic function of RU-486 has been shown with PR. Thus, a detailed analysis of the differences between the structures of GR bound to dexamethasone compared to RU-486 is of importance to understand how the ligand exerts different biological functions through one single receptor protein. This also shows that ligand binding is crucial to an understanding of the function of GR.

#### PRODUCTION OF GLUCOCORTICOID RECEPTOR CRYSTALS AND THEIR APPLICATION

The present inventors have been able to isolate, differentiate and produce crystals for the glucocorticoid receptor. Further, the differences between the GR and AR, ER, or PR receptors has been determined and, using these differences, the ability of a ligand to bind to the GR receptor or to either AR, ER, or PR can be predicted.

Preferably, the crystal is produced from a sequence comprising at least 150 amino acids, and preferably at least two hundred amino acids of GR. Preferably, the sequence comprises at least a portion of the ligand binding domain of GR. More preferably, the sequence comprises the whole ligand binding domain of GR.

Advantageously, the crystals have a resolution determined by X-ray crystallography of less than 3.6 Å and most preferably less than 2.9 Å. Preferably crystals grown using RU-486 have an effective resolution of lower than 2.9 Å.

The production of such crystals has enabled the three dimensional structure of the ligand binding domain of GR to be mapped. Use of such crystals in conjunction with the map enables a better understanding of how RU-486 and other anti-glucocorticoids bind to GR with precision. This technique can also enable the design of receptor selective glucocorticoid agonists and antagonists since now the precise differences in the binding sites between GR and the closely related AR, ER, and PR structures is now known.

Crystals of the GR binding domain can be used as models in methods for the design of synthetic compounds intended to bind to the receptor. Such models show why very slight differences in chemical moieties of a ligand potentially have widely varying binding affinities. Hence, the three dimensional structure of the ligand binding domain can be used a pharmaceutical model for compounds which bind to glucocorticoid receptors.

Embodiments of the invention will now be described in more detail, by way of example, with reference to the accompanying drawing.

Figure 1 shows modifications to the steroid nucleus to enhance its affinity for GR.

Figure 2 shows representative portions of a 2.8Å resolution SigmaA weighted 2 **Fobs-Fcalc** map where **Fobs** are the observed and **Fcalc** are the calculated structure-factor amplitudes and 2**Fobs-Fcalc** is the difference Fourier synthesis electron density map in which model error is reduced and electron density at the chosen contour (mesh diagram) approximates the molecular surface for the Ru-486-GR-LBD complex. The structure of RU-486 (tube diagram) is fitted to the experimental electron density (mesh diagram);

Figure 3 shows the GR3 crystal. The two crystallographic identical molecules are

coloured gray and dark gray.

Figure 4. Stereo picture showing the super position of GR1 (black) and GR2 (gray) and the binding of three RU-486 molecules in the asymmetric unit in the GR2 crystal form. The third RU-486 molecule in the GR 2 structure binds in the same vicinity as the approximate helix 9 position in the GR 1 structure.

Figure 5. Showing the superposition of the GR 3-dimer (light gray) and a PR monomer (black). Helix 9 undertakes a large conformational change of from the supposed agonistic position like in the PR-structure to the antagonist position in GR3. Helix 9 swings out and finds binding in a part of the coactivator pocket of an NCS molecule.

Figure 6. The dimer interface of the GR2 structure (light gray) shows that the helix 7 of the NCS molecule packs perpendicular to the N-terminal part of the NR-box II-peptide bound to the coactivator pocket in the 3ERD structure (black).

Figure 7 shows the human GR amino acid sequence aligned with the GR1, GR2 and GR3 sequences. Structural elements for the GR ligand binding domain are also shown.

#### **DNA construction work**

The human glucocorticoid receptor sequence is publicly available with accession number P04150 (SwissProt.) (Hollenberg, S. M. et al., Nature, 318: 635-41 (1985)) Over 40 different constructions have been made over the years with the goal to obtain a structure from a protein that was stable enough for crystallization and which had a fully liganded pocket and contained at least the ligand binding domain (LBD) as deduced from sequence alignment. A purification tag containing six histidine residues was also introduced at either the N- or the C-terminus with the possibility to remove by thrombin treatment.

### **Virus preparation**

Two systems were used to create the recombinant AcNPV: BacVector (Novagen, USA) and Bac-To-Bac (Invitrogen, USA). Transfection was performed according to the manufacturers' protocols. The virus was scaled up in two steps to achieve a high titer virus stock. The virus titre was determined by a plaque assay (HyQ Bevs PlaKit, HyClone, USA).

### **Protein production**

GR was recombinantly expressed using Bacculo virus infected insect cells. *Spodoptera frugiperda* (Sf9) cells (Invitrogen, USA) were maintained as suspension cultures in shake flasks and routinely passaged every third day. The serum-free medium, Sf900II (Invitrogen) was used with the addition of Gentamicin (15 mg mL<sup>-1</sup>, Sigma-Aldrich). Two stirred tank reactors (Belach Bioteknik AB, Sweden), 20 and 100 L, were used for large-scale expression. Inoculum was prepared in stirred tank reactors, 3-10 L, (Belach Bioteknik AB, Sweden). The cells were cultured in Sf900II supplemented with Gentamicin (15 mg mL<sup>-1</sup>, Sigma-Aldrich), Pluronic F-68 (0.1%, Sigma-Aldrich) and Antifoam C (12ppm, Sigma-Aldrich). pH was monitored but not adjusted. The DOT was maintained at 40% by surface aeration at 3 L min<sup>-1</sup> (20L) and 5 L min<sup>-1</sup> (100L) and intermittent purging with of oxygen at 200mL min<sup>-1</sup>. The inoculum in the fermentor was 0.7 x 10<sup>6</sup> cells mL<sup>-1</sup>. The cells were infected with a recombinant *A. californica* nuclear polyhedrosis virus, AcNPV, (Novagen, Invitrogen, USA) containing the gene encoding for the hGR-LBD at approximately 1.5- 2.0 x 10<sup>6</sup> cells mL<sup>-1</sup> at MOI 5. Dexamethasone (Sigma-Aldrich) was added at the time of infection at a concentration of 6 mM. The cells were harvested after 48 hpi and pelleted in a swing-out centrifuge at 2000 rpm, 20 min, 4°C. After centrifugation the cell pellet was frozen in N<sub>2</sub>(l) and stored at -70°C.

### **Protein purification**

Depending on expression levels 10-50 liters worth of frozen cells was disrupted by thawing in a cold degassed extraction buffer (50 mM Tris-HCl pH 8.0, 10% glycerol, 10 mM mono thioglycerol (MTG) + 50 mM dexamethasone) with a magnetic stirrer at +4°C. The ratio was kept to 2-4 x10<sup>7</sup> cells/ml extraction volume. The supernatant was

recovered after centrifugation and imidazole was added to final a concentration of 2 mM, and allowed to equilibrate with 50 ml pre-equilibrated (with extraction buffer with out MTG) Talon chelating resin (Clontech). The His-tagged GR were then allowed to batch bind to the resin during one hour of slow rotation. Non-bound protein was eluted with extraction buffer (2.5 mM MTG) until UV-baseline was reached usually after 5-10 column volumes (CV). Unspecific proteins were removed with a salt wash, 5-10 CV (10 mM Tris-HCl pH8.0, 10% glycerol, 2.5 mM MTG, 200 mM NaSCN, 50 mM dexamethasone, followed by 5-10 CV of low ionic strength buffer (10 mM Tris-HCl pH8.0, 10% glycerol, 2.5 mM MTG, 50 mM dexamethasone). The GR was then batch eluted at 4 ml/min with 10 mM Tris-HCl pH8.0, 10% glycerol, 2.5 mM MTG, 50 mM imidazole and 50 mM dexamethasone. The Histidine-tag was removed by thrombin (10U/mg GR) cleavage overnight at +4°C. The cleaved protein was loaded on a Resource 30 Q cation exchange column (Amersham Biosciences, Sweden), equilibrated in A-buffer; 10 mM Tris-HCl pH 8.2, 10% glycerol, 2.5 mM DTT, 50 mM dexamethasone and subsequently eluted in a KCl gradient.

#### **Ligand exchange**

The pure protein was dialyzed (Slide-A-Lyzer, Pierce, USA) over 48 hours at +4°C against a 2x600 ml buffer containing 10 mM Tris-HCl pH 8.5-pH8.8, 2.5 mM DTT and 50 mM RU-486. GR was finally concentrated to 5-8 mg/ml in a Centriprep-30 (Millipore) for crystallization. Protein that was not immediately used was flash frozen in liquid nitrogen in 50 ml aliquots but the best crystals were obtained from fresh material.

#### **Protein quality analysis**

To elucidate the homogeneity of GR, throughout the purification samples were collected and run on SDS and native PAGE gels (Phast, Amersham Biosciences, Sweden). Reverse phase HPLC runs were performed on a Waters HPLC system (Waters, USA) at denaturing conditions. Typically, 100 µl sample was acidified by addition of 10% acidic acid (final concentration). A sample was injected and eluted in a 25-75% acetonitrile-water gradient in 0.1% trifluoroacetic acid at 1 ml/min. The method proved to be very useful to reveal problems with ligand binding and GR

stability and for determine the concentration and GR-ligand ratio.

### **Crystallization and data collection**

Three crystal forms have been identified. The structure was first solved in the orthorhombic crystal lattice  $P2_12_12_1$  to 3.5Å resolution. Later a hexagonal lattice,  $P6_3$ , was found which diffracted to better than 2.8Å and the crystallization was reproducible. The third crystal form is from another orthorhombic form  $P2_12_12$ , which diffracts to better than 2.8Å. Despite the problems with refining GR1 and GR2 important conclusions can be drawn using information from all three structures.

### **The $P2_12_12_1$ crystals – GR 1**

The DNA construct for these crystals (GR 1) includes the part of the GR sequence as shown in Table 1. The pure protein was ultra centrifuged for 15 minutes at maximum speed in a Beckman ultracentrifuge prior to crystallization. Crystals grow in 1-15% PEG 8000, 0.05-0.1 M  $\text{CaCl}_2$  and Tris pH 8.8 at 4°C. The crystals appear after less than a week and grow to a maximum size of 60x10x2 mm in heavy precipitate. Despite the very thin size they diffract to about 3Å at 17-ID at IMCA APS with a 30 second exposure. The crystals belong to the orthorhombic lattice,  $P2_12_12_1$ , with cell dimensions  $a=67.3$   $b=87.4$   $c=93.1$  and have two molecules in the asymmetric unit. A collected data set was indexed and merged in HKL2000 (Otwinowski, Z. and M. W. (1997). Processing of X-ray diffraction data collected in oscillation mode. Methods in Enzymology. C. W. J. Carter and S. R.M. New York, Academic Press. 276.). The data is with 2 I/Sigma reflections to only 3.2 Å with a Rmerge of > 40% in the outer shell (Table 1). The structure was used initially before other data sets were available. The GR 1 coordinates are presented below.

Oscillation mode was as defined in Otwinoski, Z and M.W. (1997) Supra.

### **The $P6_3$ crystals – GR 2**

The DNA construct for these crystals (GR 2) includes the part of the GR sequence as shown in Table 1. The pure protein was treated with enterokinase before

concentration to enzymatically remove helix 12 that was disordered in the  $P2_12_12_1$  structure. GR crystals were obtained using standard vapor diffusion methods by mixing equal amounts of GR at 6 mg/ml and well solutions (1-1.5 M 1,6-hexanediol, 50 mM sodium citrate pH 5-6, 2 mM DTT at 12°C). The crystals grow as hexagonal rods in light precipitate over a period no longer than 3 weeks to a maximum size of 250x50x20 mm. The crystals were flash-cooled with the addition of 20% glycerol. On 17-ID IMCA-CAT beam line at Advanced Photon Source (APS) (Argonne National Laboratories), and a 10-second exposure, reflections could be seen to 2.5 Å on the attached ADSC Q-210 CCD detector. Several complete data sets to 2.8 Å resolution could be collected and indexed in Mosflm6.11c (CCP4) and scaled in Scala (CCP4) (Table 1). The data was used to 2.8 Å in subsequent refinement. The GR 2 coordinates are presented below.

### The $P2_12_12_1$ crystals – GR 3

The DNA construct for these crystals (GR 3) includes the part of the GR sequence as shown in Table 1. This DNA construct contain three mutations. Asn517Asp to prohibit deamidation (data not shown) and the Phe602Ser mutant, which has been reported to stabilize GR for *E. coli* expression (Garabedian, M.J. & Yamamoto, K.R. Genetic dissection of the signaling domain of a mammalian steroid receptor in yeast. *Mol Biol Cell* 3, 1245-57. (1992).). Although we have not been able to verify this, nevertheless the construct also produced 2-3 times more protein in the Bacculo virus expression system as well (2-8 mg/liter). The third mutant is Cys638Asp, a surface exposed cysteine that impose problems during purification. An aspartic acid in that position helps to solubilize the GR protein. This crystal form was also crystallized at 12°C but in 15% PEG 8000, 900 mM 1,6-hexanediol, 600 mM NaSCN, 100 mM Tris pH 8.2. The crystals grow as rods to a maximum dimension of 280x80x80 mm. One crystal was cryo cooled using the well solution but with 20% PEG 8000 and 15% ethylene glycol. A complete data set to 2.8 Å resolution was collected using a rotary anode source and the data was integrated in Mosflm and scaled in Scala (Table 1). The crystal belongs to the orthorhombic system  $P2_12_12_1$  with the cell dimensions  $a=74.5$   $b=109.7$   $c=39.1$  and has one molecule in the asymmetric unit. The GR 3 coordinates are presented below.

## Structure determination and refinement

### GR 1

The first structure was solved by molecular replacement in CNX (Brünger, A. T., P. D. Adams, *et al.* (1998). "Crystallography & NMR system: A new software suite for macromolecular structure determination." Acta Crystallogr D Biol Crystallogr 54(Pt 5): 905-21.) using a PR monomer as the search model (Williams, S. P. and P. B. Sigler (1998). "Atomic structure of progesterone complexed with its receptor." Nature 393(6683): 392-6.). Only one rotation function peak was found and a self-rotation map was quite flat. On a translation search, two solutions were above the background. The two monomers in the asymmetric unit are translationally related. This is in accordance with ultra centrifugation studies indicating that GR-LBD is a monomer in solution.

After several rounds of refinement in CNX and utilizing density modification methods like solvent flattening and NCS averaging in DM (Cowtan (1994), Newsletter on Crystallography, 31, pages 34-38), the crystallographic Rfactor was still 35% with an Rfree of 45%. Positive density in fofc maps show without doubt electron density for the ligand RU-486 and also some traces of helix 12.

### GR 2

The second crystal form was solved by molecular replacement in Molrep (Vagin, A. & Teplyakov, A. MOLREP: an automated program for molecular replacement. *J. Appl. Cryst.* 30, 1022-1025 (1997)), using the P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub> model without helix 12. Two molecules were found in the asymmetric unit related by a two fold axes. Standard procedure involving rigid body and subsequent refinement in CNX involving Torsion angle dynamics, slow cool and restrained B factor refinement utilizing restrained NSC two fold averaging. The Rfactor was 26.6% with an Rfree of 32.3%. Initial maps showed very nice density for most of the protein and particular the RU-486 molecule.

**GR 3**

The third crystal form was solved in Molrep, using a model without helix12. One giant peak appeared in the rotation function map. A systematic search in the translation function revealed that the  $P2_21_2$  solution that stuck out with R 52 % and a CC 34%. After transformation to the standard setting in  $2_12_12$ , refinement was started in CNX. The Rfactor dropped during the initial round of rigid body, B-factor and refinement to 39% without any manual model building. RU-486 ligands were included in the CNX refinement by building the necessary libraries using XPLO2D (Kleywegt, G. J. (1995). "Dictionaries for heteros." CCP4/ESF-EACBM Newsletter on Protein Crystallography 31: 45-50.). During the iterative refinement round the missing part of residues after 738-777 was built with the Grab\_build command introduced in O version 8.04 (Jones, T. A., J. Y. Zou, et al. (1991). "Improved methods for building protein models in electron density maps and the location of errors in these models." Acta Crystallogr. A 47: 110-119.).

In the crystal structure GR 3 (Figure 3) an intermolecular disulphide is formed between the 2-fold symmetry related Cys736. Helix 12 from one molecule binds perpendicular to the coactivation pocket a neighbouring molecule

**Structure description**

The overall structure is similar to that of the Progesterone receptor (PR, (Williams, S. P. and P. B. Sigler (1998) Nature 393(6683): 392-6.) but important differences can be seen especially the antagonist induced conformational change after residue Asn734. The two structures can be superimposed ) with and r.m.s fit on C-alpha of 0.975 Å for residues GR530-734 and PR686-889. The aligned structures share a 56.2% sequence identity. In the GR 3 structure, clear electron density (Figure 2) can be seen from most of the amino acid range from 530 to 777 of the full-length receptor sequence. There is one missing loop 759-767 after helix 12. The loop between helix 10 and helix 11 is poorly defined in the electron density map.

### **The structure without Helix 9**

Since antagonized (GR) protein has a less rigid C-terminus which increases the difficulties to form crystals and no protein could be recovered on shorted constructs without helix 9, enterokinase was used to remove helix 9. On binding of RU-486 helix 9 becomes displaced and enterokinase sensitive. Complete removal of helix 9 could be accomplished on a few hours of cleavage at +4°C. With an agonist bound to GR (e.g. dexamethasone), the protein was only partly cleaved by enterokinase and only after a several days at +4°C (data not shown). Again the overall structure is similar to PR with the same arrangement of helices. Part of the coactivator pocket is occupied by helix 7 from the NCS molecule (FIG 6.). Helix 7 is bound approximately perpendicular to the first turn of the coactivator peptide helix from the ER-TIF complex structures (3ERD, ). In the structure, clear density was seen for a third RU-486 molecule bound in-between the NSC protein molecules in Van der Wahl's contact with the two other correctly bound RU-486 molecules (FIG 4.). The protein was crystallized in excess of RU-486 ligands. The C17 extension of the third ligand reaches towards the hydrophobic part of the coactivator pocket.

### **The whereabouts of Helix 9 and the C-terminus**

Many models have been published of GR based on PR agonist structure (see e.g. Ray, D. W., C. S. Suen, *et al.* (1999) *Mol Endocrinol* 13(11): 1855-63.) But to model an antagonist conformation is much more difficult due to the large conformational change of helix 9 that could be seen in for example the ER raloxifene structure (Brzozowski, A. M., A. C. Pike, *et al.* (1997) *Nature* 389(6652): 753-8.). To function as an antagonist the only criteria is that helix 9 must be displaced and somehow prohibit binding of the coactivator. There does not seem to be a general way to antagonize a nuclear hormone receptor making it almost impossible to model without access of direct structural data.

The dimethylaniline side chain of RU-486 prohibits binding of helix 9 in the agonist position as seen in the PR structure. Instead helix 7 is shortened and stretched out starting with the residue of the internal Cys636 whose side chain which swings or

rotates out to the surface. Interestingly an intermolecular disulphide is formed within the crystal lattice with 2-fold symmetry related cysteine from a neighboring molecule which thereby rigidifies the loop between helix 7 and helix 7a (Figure 3). The distance between the two sulphur atoms is 2.5Å. Helix 9 enters the same symmetry molecule and binds in a cavity in-between the agonist position of helix 9 from the PR structure and the coactivator pocket revealed by the ER-alpha TIF2 structures (Pike, A.C., Brzozowski, A.M. & Hubbard, R.E. *J Steroid Biochem Mol Biol* **74**, 261-8. (2000).). But the orientation of GR helix 9 is the opposite of that of PR helix 12 (FIG 5). To our surprise a long stretch of electron density was seen on the surface between helix 6 and 7. The origin was no doubt from amino acid origin. This stretch of 10 residues matched perfectly the position of the C-terminus of PR, showing that this conformation can also be seen in an antagonized structure. This means that Helix 9 enters the neighboring molecule and the remaining part of the protein folds back and returns with the C-terminus to its parent molecule. This tail seems to be important in stabilizing the GR protein. Constructs with shorter C-terminus showed no or very low expression levels.

Table 1. Summary of data collection, processing and refinement of the three GR crystals forms.

Structure name	GR1	GR2	GR3
Construct	JY142, JY158	MF7, JY178, JY189	JY179
Sequence	500-777	519-744 <sup>1</sup>	500-777
Mutants	C638D	C638D	N517D, F602S, C638D
Space group; mol/au	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> ;2	P6 <sub>3</sub> ; 2	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> ; 1
X-ray source	17-ID IMCA-CAT	17-ID IMCA-CAT	Rotating anode
Detector	MAR-CCD	ADSC Q-210	MAR 345 image plate
Wave length (Å)	1.00	1.00	1.54
Temperature (K)	100	100	100
Resolution (Å)	48-3.5Å	48-2.8Å	40-2.8Å
Unit-cell parameters (Å)	a=67.3, b=87.4, c=93.1	a=b=132.1, c=53.0	a=74.5, b=109.7, c=39.1
Protein content (%)	53	59	47
Total number of reflections	n/a	79024	83279
No. of unique reflections	9502	13168	8219
Completeness (%)	95	100, (80) <sup>2</sup>	98.1 (98.0) <sup>1</sup>
I/σ	n/a	5.3 (1.2) <sup>3</sup>	6.7 (2.1) <sup>2</sup>
Redundancy	n/a	6.0	4.6
Rsym (%)	21.0(42.7) <sup>2</sup>	13.1 (61.1) <sup>2</sup>	10.6 (34.8) <sup>2</sup>
PVC <sup>4</sup> (%)	n/a	17.2 (80.6) <sup>2</sup>	14.0 (49.0) <sup>2</sup>
Wilson B (Å <sup>2</sup> )	n/a	77	43
Mosaicity (°)	0.5	0.5	0.6
Number of atoms in a.u.:			
Protein	3594	3383	1952
Ligand	64	96	32
Water	n/a	2	21
Hexanediol	n/a	0	24
Final Rfactor/Rfree (%)	34.4 (46.8)	26.6 (32.2)	22.8 (26.3)

<sup>1</sup> C-terminal end after enterokinase digestion.<sup>2</sup> Low resolution bin due to overloads.<sup>3</sup> Highest resolution bin.<sup>4</sup> Pooled coefficient of variation relative to overall mean (Diederichs, K. & Karplus, P.A. Improved R-factors for diffraction data analysis in macromolecular crystallography. *Nat Struct Biol* 4, 269-75 (1997).)

### Crystals of GR-LBD with an Agonist

The crystal structure of the ligand binding domain of human glucocorticoid receptor in complex with agonist Dexamethasone and a coactivator peptide (TIF2 NR-box3) has been determined and refined to 2.8 Å resolution.

### **DNA construction work**

Over 40 different constructions have been made over the years with the goal to obtain a protein that was stable enough for crystallization and which had a fully liganded pocket and contained at least the ligand binding domain (LBD) as deduced from sequence alignment. A purification tag containing six residues was also introduced at either the N- or the C-terminus with the possibility to remove by thrombin treatment.

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Two stirred tank reactors (Belach Bioteknik AB, Sweden), 20 and 100 L, were used for large-scale expression. Inoculum was prepared in stirred tank reactors, 3-10 L, (Belach Bioteknik AB, Sweden). The cells were cultured in Sf900II supplemented with Gentamicin (15 µg mL<sup>-1</sup>, Sigma-Aldrich), Pluronic F-68 (0.1%, Sigma-Aldrich) and Antifoam C (12ppm, Sigma-Aldrich). pH was monitored but not adjusted. The DOT was maintained at 40% by surface aeration at 3 L min<sup>-1</sup> (20L) and 5 L min<sup>-1</sup> (100L) and intermittent sparging of oxygen at 200 mL min<sup>-1</sup>. The inoculum in the

fermentor was  $0.7 \times 10^6$  cells  $\text{mL}^{-1}$ . The cells were infected with a recombinant *A. californica* nuclear polyhedrosis virus, AcNPV, (Novagen, Invitrogen, USA) containing the gene encoding for the hGR-lbd at approximately  $1.5\text{-}2.0 \times 10^6$  cells  $\text{mL}^{-1}$  at MOI 5. Dexamethasone (Sigma-Aldrich) was added at the time of infection at a concentration of 6  $\mu\text{M}$ . The cells were harvested after 48 hpi and pelleted in a swing-out centrifuge at 2000 rpm, 20 min, 4°C. After centrifugation the cell pellet was frozen in  $\text{N}_2(1)$  and stored at 70°C.

### Protein purification

Depending on expression levels 10-50 litres worth of frozen cells was disrupted by thawing in a cold degassed extraction buffer (50 mM Tris-HCl pH 8.0, 10% glycerol, 10 mM mono thioglycerol (MTG) + 50  $\mu\text{M}$  dexametasone) with a magnetic stirrer at +4°C. The ratio was kept to  $2\text{-}4 \times 10^7$  cells/ml extraction volume. The supernatant was recovered after centrifugation and one wash step and poured into a 1-litre flask with the addition of imadazole to final a concentration of 2 mM and 50 ml a pre-equilibrated (with extraction buffer without MTG) Talon chelating resin (CloneTech). The His-tagged GR were then allowed to batch bind to the resin during one hour of slowly rotation. This step was crucial for speed and to have an even distribution of GR in the resin. The slurry was briefly centrifugated 700 x g for 2 minutes and most of the supernatant was discarded. The matrix was transferred to an XK50 column (Amersham-Pharmacia Biotech) and manually packed in the cold room with the high flow rate given by the gravity. Non-bound protein was eluted with extraction buffer (2.5 mM MTG) until UV-baseline was reached usually after 5.10 column volumes (CV). Unspecific proteins were removed with a salt wash, 5-10 CV (10 mM Tris-HCl pH8.0, 10% glycerol, 2.5 mM MTG, 200 mM NaSCN, 50  $\mu\text{M}$  dexametasone, followed by 5-10 CV of low ionic strength buffer (10 mM Tris-HCl pH8.0, 10% glycerol, 2.5 mM MTG, 50  $\mu\text{M}$  dexametasone). The XK50 column was then connected to an FPLC-system (Amersham-Pharmacia Biotech) at +4°C. The GR was then batch eluted at 4 ml/min with 10 mM Tris-HCl pH8.0, 10% glycerol, 2.5 mM MTG, 50 mM imidazole and 50  $\mu\text{M}$  dexametasone. The Histidine-tag was removed by thrombin (10U/mg GR) cleavage overnight at +4°C. The cleaved protein was loaded on a Resource 30 Q cation exchange column (Amersham-Pharmacia

Biotech). The GR was washed at 1 ml/min in A-buffer; 10 mM Tris-HCl pH 8.2, 10% glycerol, 2.5 mM DTT, 50  $\mu$ M dexametasone and subsequently eluted in a KCl gradient. The main peak was collected, at ~100-125 mM KCl, and diluted one time with the A-buffer without ligand and concentrated with a Centriprep-30 (MilliPore) to 8-40 mg/ml.

#### **Crystallization, data collection and structure solution**

Crystals were grown using hanging drop vapor diffusion methods. By mixing 1:1 of protein with the presence of TIF2 NR-box 3 peptide with well solution containing, 10-15% PEG550 MME, 0.1-0.2 M MgCl and Hepes pH 7.6. Crystal were grown at 10°C and appeared after 1 day and grew over a week to maximum dimension of 100x100x50 micrometer. Crystals were flash cooled in liquid nitrogen gas stream with the addition of extra PEG550 MME. A full dataset to 2.8Å could be collected on ID14-4 beamline at ESRF, France. The data was indexed and processed in Mosflm and scaled in Scala.

The crystals belong to the triclinic space group  $P3_1$  with a pair of dimers in the asymmetric unit. The solvent content is 65% and cell dimensions are  $a=b=127.4$ ,  $c=91.8$ ,  $\alpha=\beta=90^\circ$ ,  $\gamma=120^\circ$ . The structure was solved by molecular replacement using Molrep and a model based on the coordinates of the antagonist form of GR-LDB solved at Karo Bio previously, together with the N-terminal part of the progesterone receptor.

## ANNEX

## GR 1

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REMARK coordinates from simulated annealing refinement
REMARK refinement resolution: 20.0 - 3.2 Å
REMARK starting r= 0.3642 free_r= 0.4500
REMARK final r= 0.3436 free_r= 0.4685
REMARK rmsd bonds= 0.009741 rmsd angles= 1.63529
REMARK wa_initial= 14.7646 wa_dynamics= 16.8608 wa_final= 18.2355
REMARK target= mlf md-method= torsion annealing schedule= slowcool
REMARK starting temperature= 3500 total md steps= 140 * 6
REMARK sg= P2(1)2(1)2(1) a= 67.331 b= 87.423 c= 93.109 alpha= 90.000 beta= 90.000
gamma= 90.000
REMARK parameter file 1 : MSI_CNX_TOPPAR:protein_rep.param
REMARK parameter file 2 : MSI_CNX_TOPPAR:water_rep.param
REMARK parameter file 3 : MSI_CNX_TOPPAR:ion.param
REMARK molecular structure file: gen.mtf
REMARK input coordinates: ../Quanta/x3in.pdb
REMARK reflection file= gr31401c.cv
REMARK ncs= restrain ncs file= ncs2.def
REMARK B-correction resolution: 6.0 - 3.2
REMARK warning: B-correction gave atomic B-values less than zero
REMARK they have been reset to zero
REMARK B-factor correction applied to coordinate array B: -1.232
REMARK bulk solvent: (Mask) density level= 0.323811 e/Å3, B-factor= 40.0116 Å2
REMARK reflections with |Fobs|/sigma F < 0.0 rejected
REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
REMARK theoretical total number of refl. in resol. range: 9452 ( 100.0 % )
REMARK number of unobserved reflections (no entry or |F|=0): 1105 ( 11.7 % )
REMARK number of reflections rejected: 0 ( 0.0 % )
REMARK total number of reflections used: 8347 ( 88.3 % )
REMARK number of reflections in working set: 7481 ( 79.1 % )
REMARK number of reflections in test set: 866 ( 9.2 % )
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REMARK DATE=Mar-23-2001 17:22:01 created by user: jakobc
REMARK Written by CNX VERSION:2000
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ATOM 3 CG2 THR A 531 15.970 83.353 9.802 1.00 9.76 A C
ATOM 4 C THR A 531 18.675 81.742 7.570 1.00 9.15 A C
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ATOM 11 CG LEU A 532 23.313 80.775 7.817 1.00 11.09 A C
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ATOM 13 CD2 LEU A 532 24.471 81.696 7.474 1.00 12.26 A C
ATOM 14 C LEU A 532 20.991 79.900 9.503 1.00 7.70 A C
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ATOM 32 CG LEU A 535 20.156 76.496 7.032 1.00 4.29 A C
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ATOM 43 C LEU A 536 19.935 73.984 11.876 1.00 6.65 A C

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ATOM	47	CB	GLU	A	537	16.852	75.350	13.374	1.00	5.84	A	C
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ATOM	52	C	GLU	A	537	17.508	72.984	13.026	1.00	7.81	A	C
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ATOM	66	CD1	ILE	A	539	22.733	71.376	8.958	1.00	1.63	A	C
ATOM	67	C	ILE	A	539	20.282	69.098	11.426	1.00	7.61	A	C
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ATOM	72	CG	GLU	A	540	21.410	70.745	15.441	1.00	10.25	A	C
ATOM	73	CD	GLU	A	540	22.081	71.478	14.296	1.00	12.97	A	C
ATOM	74	OE1	GLU	A	540	23.049	72.246	14.534	1.00	13.29	A	O
ATOM	75	OE2	GLU	A	540	21.635	71.279	13.148	1.00	13.53	A	O
ATOM	76	C	GLU	A	540	20.043	67.540	14.210	1.00	5.41	A	C
ATOM	77	O	GLU	A	540	19.021	67.365	14.873	1.00	4.81	A	O
ATOM	78	N	PRO	A	541	20.794	66.515	13.775	1.00	4.19	A	N
ATOM	79	CD	PRO	A	541	22.118	66.600	13.126	1.00	2.90	A	C
ATOM	80	CA	PRO	A	541	20.456	65.123	14.059	1.00	3.73	A	C
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ATOM	82	CG	PRO	A	541	22.473	65.155	12.893	1.00	3.20	A	C
ATOM	83	C	PRO	A	541	19.710	64.964	15.385	1.00	3.10	A	C
ATOM	84	O	PRO	A	541	19.994	65.688	16.345	1.00	1.61	A	O
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ATOM	87	CB	GLU	A	542	16.535	63.380	16.251	1.00	3.65	A	C
ATOM	88	CG	GLU	A	542	15.440	64.127	17.060	1.00	5.77	A	C
ATOM	89	CD	GLU	A	542	14.017	63.956	16.502	1.00	6.88	A	C
ATOM	90	OE1	GLU	A	542	13.826	64.177	15.283	1.00	7.55	A	O
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ATOM	92	C	GLU	A	542	18.526	62.860	17.715	1.00	3.12	A	C
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ATOM	94	N	VAL	A	543	17.998	63.017	18.929	1.00	3.73	A	N
ATOM	95	CA	VAL	A	543	18.370	62.241	20.115	1.00	3.10	A	C
ATOM	96	CB	VAL	A	543	17.197	62.204	21.125	1.00	1.86	A	C
ATOM	97	CG1	VAL	A	543	17.264	63.376	22.090	1.00	1.42	A	C
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ATOM	102	CA	LEU	A	544	20.470	59.124	19.552	1.00	4.11	A	C
ATOM	103	CB	LEU	A	544	21.998	59.020	19.479	1.00	6.58	A	C
ATOM	104	CG	LEU	A	544	22.657	59.317	18.125	1.00	8.79	A	C
ATOM	105	CD1	LEU	A	544	24.142	58.987	18.179	1.00	8.45	A	C
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ATOM	111	CB	TYR	A	545	16.996	56.060	20.785	1.00	1.37	A	C
ATOM	112	CG	TYR	A	545	16.023	56.763	21.695	1.00	0.00	A	C
ATOM	113	CD1	TYR	A	545	16.070	56.568	23.062	1.00	0.00	A	C
ATOM	114	CE1	TYR	A	545	15.133	57.169	23.913	1.00	0.00	A	C
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ATOM	117	CZ	TYR	A	545	14.132	57.974	23.386	1.00	0.00	A	C
ATOM	118	OH	TYR	A	545	13.176	58.496	24.218	1.00	0.00	A	O
ATOM	119	C	TYR	A	545	19.281	55.021	21.140	1.00	4.25	A	C
ATOM	120	O	TYR	A	545	19.087	54.119	20.317	1.00	4.51	A	O
ATOM	121	N	ALA	A	546	20.195	54.946	22.092	1.00	2.99	A	N
ATOM	122	CA	ALA	A	546	21.039	53.784	22.245	1.00	4.16	A	C
ATOM	123	CB	ALA	A	546	22.185	54.106	23.211	1.00	4.14	A	C
ATOM	124	C	ALA	A	546	20.225	52.603	22.772	1.00	4.78	A	C

ATOM	125	O	ALA	A	546	20.339	51.472	22.289	1.00	4.10	A	O
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ATOM	127	CA	GLY	A	547	18.625	51.802	24.346	1.00	5.70	A	C
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ATOM	129	O	GLY	A	547	20.585	50.447	24.598	1.00	6.37	A	O
ATOM	130	N	TYR	A	548	19.565	51.162	26.471	1.00	6.53	A	N
ATOM	131	CA	TYR	A	548	20.488	50.519	27.389	1.00	8.77	A	C
ATOM	132	CB	TYR	A	548	20.591	51.347	28.667	1.00	9.30	A	C
ATOM	133	CG	TYR	A	548	21.785	51.065	29.567	1.00	11.60	A	C
ATOM	134	CD1	TYR	A	548	21.699	51.297	30.945	1.00	10.09	A	C
ATOM	135	CE1	TYR	A	548	22.801	51.111	31.782	1.00	9.33	A	C
ATOM	136	CD2	TYR	A	548	23.017	50.635	29.048	1.00	10.10	A	C
ATOM	137	CE2	TYR	A	548	24.132	50.447	29.885	1.00	8.65	A	C
ATOM	138	CZ	TYR	A	548	24.008	50.688	31.250	1.00	9.18	A	C
ATOM	139	OH	TYR	A	548	25.070	50.503	32.102	1.00	8.92	A	O
ATOM	140	C	TYR	A	548	19.895	49.158	27.716	1.00	9.53	A	C
ATOM	141	O	TYR	A	548	18.729	48.884	27.415	1.00	10.36	A	O
ATOM	142	N	ASP	A	549	20.701	48.292	28.317	1.00	9.86	A	N
ATOM	143	CA	ASP	A	549	20.202	46.984	28.696	1.00	8.90	A	C
ATOM	144	CB	ASP	A	549	21.354	46.089	29.173	1.00	9.09	A	C
ATOM	145	CG	ASP	A	549	22.325	45.713	28.044	1.00	8.79	A	C
ATOM	146	OD1	ASP	A	549	23.398	45.148	28.352	1.00	8.48	A	O
ATOM	147	OD2	ASP	A	549	22.022	45.973	26.855	1.00	9.18	A	O
ATOM	148	C	ASP	A	549	19.236	47.303	29.829	1.00	8.25	A	C
ATOM	149	O	ASP	A	549	18.090	46.855	29.842	1.00	7.04	A	O
ATOM	150	N	SER	A	550	19.711	48.109	30.772	1.00	8.25	A	N
ATOM	151	CA	SER	A	550	18.878	48.526	31.893	1.00	9.02	A	C
ATOM	152	CB	SER	A	550	17.669	49.317	31.347	1.00	10.47	A	C
ATOM	153	OG	SER	A	550	18.023	50.167	30.257	1.00	12.73	A	O
ATOM	154	C	SER	A	550	18.394	47.308	32.714	1.00	8.94	A	C
ATOM	155	O	SER	A	550	17.186	47.038	32.794	1.00	8.38	A	O
ATOM	156	N	SER	A	551	19.345	46.594	33.325	1.00	8.72	A	N
ATOM	157	CA	SER	A	551	19.047	45.392	34.112	1.00	8.14	A	C
ATOM	158	CB	SER	A	551	18.582	44.252	33.188	1.00	8.08	A	C
ATOM	159	OG	SER	A	551	17.427	44.598	32.441	1.00	8.70	A	O
ATOM	160	C	SER	A	551	20.261	44.910	34.919	1.00	7.95	A	C
ATOM	161	O	SER	A	551	20.142	44.595	36.110	1.00	8.58	A	O
ATOM	162	N	VAL	A	552	21.416	44.823	34.259	1.00	6.81	A	N
ATOM	163	CA	VAL	A	552	22.658	44.395	34.909	1.00	5.43	A	C
ATOM	164	CB	VAL	A	552	23.584	43.637	33.913	1.00	4.57	A	C
ATOM	165	CG1	VAL	A	552	23.446	42.122	34.111	1.00	2.85	A	C
ATOM	166	CG2	VAL	A	552	23.216	44.005	32.487	1.00	4.42	A	C
ATOM	167	C	VAL	A	552	23.421	45.600	35.492	1.00	5.91	A	C
ATOM	168	O	VAL	A	552	23.824	46.511	34.749	1.00	6.48	A	O
ATOM	169	N	PRO	A	553	23.639	45.609	36.826	1.00	6.13	A	N
ATOM	170	CD	PRO	A	553	23.548	44.413	37.686	1.00	5.59	A	C
ATOM	171	CA	PRO	A	553	24.344	46.688	37.528	1.00	5.75	A	C
ATOM	172	CB	PRO	A	553	25.045	45.948	38.658	1.00	5.99	A	C
ATOM	173	CG	PRO	A	553	24.031	44.926	39.031	1.00	5.66	A	C
ATOM	174	C	PRO	A	553	25.304	47.422	36.604	1.00	6.56	A	C
ATOM	175	O	PRO	A	553	25.875	46.820	35.692	1.00	5.64	A	O
ATOM	176	N	ASP	A	554	25.500	48.715	36.844	1.00	7.79	A	N
ATOM	177	CA	ASP	A	554	26.356	49.501	35.958	1.00	9.05	A	C
ATOM	178	CB	ASP	A	554	26.208	50.998	36.232	1.00	11.36	A	C
ATOM	179	CG	ASP	A	554	26.141	51.813	34.946	1.00	12.79	A	C
ATOM	180	OD1	ASP	A	554	26.910	51.509	34.001	1.00	14.07	A	O
ATOM	181	OD2	ASP	A	554	25.321	52.755	34.886	1.00	13.86	A	O
ATOM	182	C	ASP	A	554	27.833	49.151	35.922	1.00	8.55	A	C
ATOM	183	O	ASP	A	554	28.658	49.784	36.581	1.00	6.90	A	O
ATOM	184	N	SER	A	555	28.143	48.153	35.102	1.00	8.20	A	N
ATOM	185	CA	SER	A	555	29.495	47.659	34.908	1.00	7.64	A	C
ATOM	186	CB	SER	A	555	29.441	46.373	34.080	1.00	5.00	A	C
ATOM	187	OG	SER	A	555	28.434	45.498	34.547	1.00	1.10	A	O
ATOM	188	C	SER	A	555	30.390	48.699	34.206	1.00	8.56	A	C
ATOM	189	O	SER	A	555	30.030	49.267	33.163	1.00	8.04	A	O
ATOM	190	N	THR	A	556	31.559	48.944	34.793	1.00	8.79	A	N
ATOM	191	CA	THR	A	556	32.528	49.884	34.239	1.00	7.39	A	C
ATOM	192	CB	THR	A	556	33.842	49.894	35.097	1.00	7.41	A	C
ATOM	193	OG1	THR	A	556	34.837	50.705	34.466	1.00	6.96	A	O
ATOM	194	CG2	THR	A	556	34.392	48.484	35.269	1.00	7.68	A	C
ATOM	195	C	THR	A	556	32.821	49.452	32.802	1.00	5.72	A	C
ATOM	196	O	THR	A	556	33.531	50.138	32.071	1.00	6.36	A	O
ATOM	197	N	TRP	A	557	32.267	48.306	32.408	1.00	3.95	A	N
ATOM	198	CA	TRP	A	557	32.451	47.801	31.059	1.00	3.22	A	C
ATOM	199	CB	TRP	A	557	32.930	46.333	31.045	1.00	3.35	A	C
ATOM	200	CG	TRP	A	557	32.006	45.304	31.663	1.00	1.02	A	C
ATOM	201	CD2	TRP	A	557	30.984	44.542	30.992	1.00	0.31	A	C
ATOM	202	CE2	TRP	A	557	30.371	43.719	31.964	1.00	0.33	A	C
ATOM	203	CE3	TRP	A	557	30.524	44.480	29.668	1.00	0.00	A	C
ATOM	204	CD1	TRP	A	557	31.970	44.916	32.973	1.00	0.00	A	C
ATOM	205	NE1	TRP	A	557	30.992	43.966	33.160	1.00	0.00	A	N

ATOM	206	CZ2	TRP	A	557	29.325	42.848	31.652	1.00	0.00	A	C
ATOM	207	CZ3	TRP	A	557	29.477	43.609	29.364	1.00	0.00	A	C
ATOM	208	CH2	TRP	A	557	28.894	42.811	30.349	1.00	0.00	A	C
ATOM	209	C	TRP	A	557	31.162	47.918	30.270	1.00	3.31	A	C
ATOM	210	O	TRP	A	557	31.187	48.021	29.044	1.00	3.21	A	O
ATOM	211	N	ARG	A	558	30.031	47.925	30.968	1.00	3.04	A	N
ATOM	212	CA	ARG	A	558	28.750	48.016	30.281	1.00	2.87	A	C
ATOM	213	CB	ARG	A	558	27.622	47.457	31.161	1.00	2.86	A	C
ATOM	214	CG	ARG	A	558	26.312	47.262	30.425	1.00	4.01	A	C
ATOM	215	CD	ARG	A	558	25.333	46.423	31.220	1.00	7.57	A	C
ATOM	216	NE	ARG	A	558	25.339	45.012	30.818	1.00	12.59	A	N
ATOM	217	CZ	ARG	A	558	26.196	44.090	31.261	1.00	14.76	A	C
ATOM	218	NH1	ARG	A	558	27.140	44.417	32.138	1.00	17.10	A	N
ATOM	219	NH2	ARG	A	558	26.106	42.838	30.828	1.00	16.31	A	N
ATOM	220	C	ARG	A	558	28.469	49.455	29.870	1.00	2.65	A	C
ATOM	221	O	ARG	A	558	27.534	49.732	29.115	1.00	2.16	A	O
ATOM	222	N	ILE	A	559	29.285	50.377	30.367	1.00	2.98	A	N
ATOM	223	CA	ILE	A	559	29.125	51.778	30.001	1.00	3.70	A	C
ATOM	224	CB	ILE	A	559	29.390	52.729	31.201	1.00	4.31	A	C
ATOM	225	CG2	ILE	A	559	30.837	52.652	31.647	1.00	4.63	A	C
ATOM	226	CG1	ILE	A	559	29.072	54.167	30.791	1.00	5.80	A	C
ATOM	227	CD1	ILE	A	559	27.642	54.384	30.287	1.00	8.06	A	C
ATOM	228	C	ILE	A	559	30.082	52.108	28.852	1.00	3.12	A	C
ATOM	229	O	ILE	A	559	29.657	52.533	27.784	1.00	3.11	A	O
ATOM	230	N	MET	A	560	31.371	51.889	29.067	1.00	1.78	A	N
ATOM	231	CA	MET	A	560	32.351	52.162	28.043	1.00	0.00	A	C
ATOM	232	CB	MET	A	560	33.706	51.696	28.516	1.00	0.00	A	C
ATOM	233	CG	MET	A	560	34.065	52.360	29.819	1.00	0.00	A	C
ATOM	234	SD	MET	A	560	33.962	54.164	29.667	1.00	0.17	A	S
ATOM	235	CE	MET	A	560	35.595	54.651	30.118	1.00	0.49	A	C
ATOM	236	C	MET	A	560	31.940	51.453	26.785	1.00	0.00	A	C
ATOM	237	O	MET	A	560	32.155	51.951	25.680	1.00	1.25	A	O
ATOM	238	N	THR	A	561	31.320	50.293	26.962	1.00	0.00	A	N
ATOM	239	CA	THR	A	561	30.845	49.496	25.837	1.00	0.00	A	C
ATOM	240	CB	THR	A	561	30.312	48.143	26.320	1.00	0.00	A	C
ATOM	241	OG1	THR	A	561	31.399	47.388	26.856	1.00	0.00	A	O
ATOM	242	CG2	THR	A	561	29.665	47.366	25.173	1.00	0.00	A	C
ATOM	243	C	THR	A	561	29.732	50.244	25.118	1.00	1.27	A	C
ATOM	244	O	THR	A	561	29.903	50.726	23.994	1.00	0.00	A	O
ATOM	245	N	THR	A	562	28.584	50.332	25.780	1.00	3.02	A	N
ATOM	246	CA	THR	A	562	27.453	51.039	25.214	1.00	3.36	A	C
ATOM	247	CB	THR	A	562	26.378	51.288	26.271	1.00	2.18	A	C
ATOM	248	OG1	THR	A	562	26.121	50.077	26.983	1.00	3.18	A	O
ATOM	249	CG2	THR	A	562	25.103	51.745	25.615	1.00	3.49	A	C
ATOM	250	C	THR	A	562	27.989	52.378	24.709	1.00	3.72	A	C
ATOM	251	O	THR	A	562	27.654	52.826	23.614	1.00	4.20	A	O
ATOM	252	N	LEU	A	563	28.842	53.009	25.510	1.00	3.26	A	N
ATOM	253	CA	LEU	A	563	29.415	54.273	25.112	1.00	2.19	A	C
ATOM	254	CB	LEU	A	563	30.422	54.757	26.158	1.00	0.00	A	C
ATOM	255	CG	LEU	A	563	29.771	55.561	27.297	1.00	0.00	A	C
ATOM	256	CD1	LEU	A	563	30.765	55.820	28.414	1.00	0.00	A	C
ATOM	257	CD2	LEU	A	563	29.243	56.887	26.753	1.00	0.00	A	C
ATOM	258	C	LEU	A	563	30.064	54.065	23.759	1.00	2.77	A	C
ATOM	259	O	LEU	A	563	29.491	54.418	22.734	1.00	1.04	A	O
ATOM	260	N	ASN	A	564	31.245	53.466	23.749	1.00	2.98	A	N
ATOM	261	CA	ASN	A	564	31.952	53.210	22.503	1.00	2.64	A	C
ATOM	262	CB	ASN	A	564	32.941	52.055	22.728	1.00	0.09	A	C
ATOM	263	CG	ASN	A	564	33.722	51.690	21.481	1.00	1.80	A	C
ATOM	264	OD1	ASN	A	564	33.412	50.706	20.808	1.00	2.98	A	O
ATOM	265	ND2	ASN	A	564	34.741	52.485	21.163	1.00	1.77	A	N
ATOM	266	C	ASN	A	564	30.972	52.880	21.369	1.00	2.80	A	C
ATOM	267	O	ASN	A	564	31.149	53.287	20.223	1.00	0.93	A	O
ATOM	268	N	MET	A	565	29.921	52.148	21.712	1.00	4.69	A	N
ATOM	269	CA	MET	A	565	28.930	51.738	20.730	1.00	6.85	A	C
ATOM	270	CB	MET	A	565	27.854	50.870	21.396	1.00	6.83	A	C
ATOM	271	CG	MET	A	565	27.098	49.953	20.441	1.00	8.00	A	C
ATOM	272	SD	MET	A	565	28.139	48.642	19.708	1.00	8.84	A	S
ATOM	273	CE	MET	A	565	28.850	49.503	18.290	1.00	6.39	A	C
ATOM	274	C	MET	A	565	28.294	52.967	20.126	1.00	8.23	A	C
ATOM	275	O	MET	A	565	28.102	53.050	18.918	1.00	8.56	A	O
ATOM	276	N	LEU	A	566	27.979	53.924	20.993	1.00	8.11	A	N
ATOM	277	CA	LEU	A	566	27.341	55.177	20.603	1.00	6.27	A	C
ATOM	278	CB	LEU	A	566	26.825	55.908	21.852	1.00	4.16	A	C
ATOM	279	CG	LEU	A	566	25.742	56.981	21.694	1.00	2.52	A	C
ATOM	280	CD1	LEU	A	566	24.564	56.423	20.931	1.00	1.38	A	C
ATOM	281	CD2	LEU	A	566	25.292	57.461	23.060	1.00	1.84	A	C
ATOM	282	C	LEU	A	566	28.332	56.048	19.873	1.00	5.12	A	C
ATOM	283	O	LEU	A	566	27.963	57.004	19.224	1.00	5.30	A	O
ATOM	284	N	GLY	A	567	29.603	55.707	19.981	1.00	3.12	A	N
ATOM	285	CA	GLY	A	567	30.613	56.502	19.319	1.00	1.91	A	C
ATOM	286	C	GLY	A	567	30.390	56.590	17.833	1.00	0.39	A	C

ATOM	287	O	GLY	A	567	29.825	57.549	17.348	1.00	0.00	A	O
ATOM	288	N	GLY	A	568	30.835	55.572	17.118	1.00	0.00	A	N
ATOM	289	CA	GLY	A	568	30.709	55.539	15.679	1.00	0.00	A	C
ATOM	290	C	GLY	A	568	29.347	55.889	15.153	1.00	0.00	A	C
ATOM	291	O	GLY	A	568	29.200	56.181	13.975	1.00	0.00	A	O
ATOM	292	N	ARG	A	569	28.335	55.851	16.002	1.00	0.00	A	N
ATOM	293	CA	ARG	A	569	26.996	56.185	15.535	1.00	1.55	A	C
ATOM	294	CB	ARG	A	569	25.951	55.315	16.253	1.00	2.82	A	C
ATOM	295	CG	ARG	A	569	24.496	55.482	15.800	1.00	3.01	A	C
ATOM	296	CD	ARG	A	569	23.617	54.546	16.640	1.00	4.65	A	C
ATOM	297	NE	ARG	A	569	22.254	55.027	16.880	1.00	4.87	A	N
ATOM	298	CZ	ARG	A	569	21.572	54.770	17.992	1.00	3.85	A	C
ATOM	299	NH1	ARG	A	569	22.129	54.044	18.950	1.00	4.04	A	N
ATOM	300	NH2	ARG	A	569	20.346	55.242	18.157	1.00	3.24	A	N
ATOM	301	C	ARG	A	569	26.792	57.671	15.807	1.00	1.55	A	C
ATOM	302	O	ARG	A	569	26.120	58.349	15.053	1.00	1.41	A	O
ATOM	303	N	GLN	A	570	27.389	58.165	16.889	1.00	1.31	A	N
ATOM	304	CA	GLN	A	570	27.315	59.570	17.233	1.00	2.14	A	C
ATOM	305	CB	GLN	A	570	27.816	59.821	18.659	1.00	4.40	A	C
ATOM	306	CG	GLN	A	570	26.770	59.652	19.758	1.00	5.78	A	C
ATOM	307	CD	GLN	A	570	27.221	60.189	21.124	1.00	7.26	A	C
ATOM	308	OE1	GLN	A	570	27.564	61.368	21.273	1.00	7.79	A	O
ATOM	309	NE2	GLN	A	570	27.213	59.322	22.125	1.00	6.81	A	N
ATOM	310	C	GLN	A	570	28.219	60.283	16.234	1.00	3.00	A	C
ATOM	311	O	GLN	A	570	28.100	61.482	16.024	1.00	5.91	A	O
ATOM	312	N	VAL	A	571	29.129	59.539	15.617	1.00	4.20	A	N
ATOM	313	CA	VAL	A	571	30.044	60.091	14.613	1.00	5.32	A	C
ATOM	314	CB	VAL	A	571	31.309	59.196	14.450	1.00	5.65	A	C
ATOM	315	CG1	VAL	A	571	31.974	59.431	13.100	1.00	5.90	A	C
ATOM	316	CG2	VAL	A	571	32.293	59.497	15.565	1.00	6.42	A	C
ATOM	317	C	VAL	A	571	29.340	60.199	13.259	1.00	5.55	A	C
ATOM	318	O	VAL	A	571	28.856	61.259	12.882	1.00	4.21	A	O
ATOM	319	N	ILE	A	572	29.287	59.090	12.534	1.00	4.66	A	N
ATOM	320	CA	ILE	A	572	28.646	59.045	11.230	1.00	2.63	A	C
ATOM	321	CB	ILE	A	572	28.245	57.576	10.864	1.00	1.46	A	C
ATOM	322	CG2	ILE	A	572	29.315	56.612	11.317	1.00	0.95	A	C
ATOM	323	CG1	ILE	A	572	26.943	57.177	11.535	1.00	2.22	A	C
ATOM	324	CD1	ILE	A	572	25.747	57.476	10.684	1.00	3.33	A	C
ATOM	325	C	ILE	A	572	27.407	59.942	11.195	1.00	1.14	A	C
ATOM	326	O	ILE	A	572	27.118	60.575	10.186	1.00	1.64	A	O
ATOM	327	N	ALA	A	573	26.686	59.997	12.309	1.00	0.00	A	N
ATOM	328	CA	ALA	A	573	25.476	60.799	12.402	1.00	0.00	A	C
ATOM	329	CB	ALA	A	573	24.770	60.553	13.706	1.00	0.00	A	C
ATOM	330	C	ALA	A	573	25.790	62.246	12.297	1.00	0.35	A	C
ATOM	331	O	ALA	A	573	24.888	63.053	12.166	1.00	1.60	A	O
ATOM	332	N	ALA	A	574	27.075	62.562	12.376	1.00	2.50	A	N
ATOM	333	CA	ALA	A	574	27.558	63.932	12.301	1.00	2.87	A	C
ATOM	334	CB	ALA	A	574	28.622	64.172	13.365	1.00	2.23	A	C
ATOM	335	C	ALA	A	574	28.123	64.213	10.920	1.00	2.36	A	C
ATOM	336	O	ALA	A	574	27.706	65.154	10.264	1.00	2.71	A	O
ATOM	337	N	VAL	A	575	29.072	63.400	10.479	1.00	1.01	A	N
ATOM	338	CA	VAL	A	575	29.664	63.588	9.163	1.00	1.65	A	C
ATOM	339	CB	VAL	A	575	30.230	62.284	8.626	1.00	1.37	A	C
ATOM	340	CG1	VAL	A	575	31.347	62.565	7.654	1.00	0.00	A	C
ATOM	341	CG2	VAL	A	575	30.668	61.416	9.768	1.00	0.00	A	C
ATOM	342	C	VAL	A	575	28.633	64.088	8.152	1.00	3.13	A	C
ATOM	343	O	VAL	A	575	28.944	64.923	7.310	1.00	3.49	A	O
ATOM	344	N	LYS	A	576	27.407	63.572	8.230	1.00	4.74	A	N
ATOM	345	CA	LYS	A	576	26.349	63.981	7.310	1.00	5.56	A	C
ATOM	346	CB	LYS	A	576	25.142	63.058	7.411	1.00	6.56	A	C
ATOM	347	CG	LYS	A	576	24.059	63.349	6.383	1.00	7.51	A	C
ATOM	348	CD	LYS	A	576	22.681	63.455	7.042	1.00	8.62	A	C
ATOM	349	CE	LYS	A	576	22.487	64.808	7.718	1.00	8.32	A	C
ATOM	350	NZ	LYS	A	576	22.640	65.931	6.743	1.00	7.57	A	N
ATOM	351	C	LYS	A	576	25.909	65.386	7.659	1.00	4.91	A	C
ATOM	352	O	LYS	A	576	25.764	66.234	6.781	1.00	4.32	A	O
ATOM	353	N	TRP	A	577	25.675	65.621	8.949	1.00	3.15	A	N
ATOM	354	CA	TRP	A	577	25.268	66.940	9.421	1.00	1.03	A	C
ATOM	355	CB	TRP	A	577	25.164	66.956	10.939	1.00	0.00	A	C
ATOM	356	CG	TRP	A	577	25.096	68.343	11.487	1.00	0.00	A	C
ATOM	357	CD2	TRP	A	577	26.195	69.115	11.970	1.00	0.66	A	C
ATOM	358	CE2	TRP	A	577	25.682	70.369	12.368	1.00	0.00	A	C
ATOM	359	CE3	TRP	A	577	27.569	68.868	12.106	1.00	1.55	A	C
ATOM	360	CD1	TRP	A	577	23.987	69.139	11.604	1.00	0.00	A	C
ATOM	361	NE1	TRP	A	577	24.332	70.357	12.134	1.00	0.00	A	N
ATOM	362	CZ2	TRP	A	577	26.498	71.375	12.895	1.00	1.32	A	C
ATOM	363	CZ3	TRP	A	577	28.378	69.867	12.629	1.00	2.05	A	C
ATOM	364	CH2	TRP	A	577	27.840	71.108	13.018	1.00	1.38	A	C
ATOM	365	C	TRP	A	577	26.327	67.938	8.991	1.00	0.05	A	C
ATOM	366	O	TRP	A	577	26.022	69.053	8.585	1.00	0.00	A	O
ATOM	367	N	ALA	A	578	27.578	67.503	9.082	1.00	1.14	A	N

ATOM	368	CA	ALA	A	578	28.727	68.313	8.734	1.00	2.23	A	C
ATOM	369	CB	ALA	A	578	29.977	67.648	9.240	1.00	1.79	A	C
ATOM	370	C	ALA	A	578	28.840	68.594	7.239	1.00	3.61	A	C
ATOM	371	O	ALA	A	578	29.738	69.312	6.811	1.00	3.99	A	O
ATOM	372	N	LYS	A	579	27.934	68.021	6.450	1.00	4.48	A	N
ATOM	373	CA	LYS	A	579	27.903	68.241	4.997	1.00	5.13	A	C
ATOM	374	CB	LYS	A	579	27.792	66.911	4.237	1.00	4.34	A	C
ATOM	375	CG	LYS	A	579	29.108	66.170	4.071	1.00	5.17	A	C
ATOM	376	CD	LYS	A	579	28.916	64.825	3.407	1.00	4.91	A	C
ATOM	377	CE	LYS	A	579	28.297	63.816	4.374	1.00	5.38	A	C
ATOM	378	NZ	LYS	A	579	29.213	63.431	5.492	1.00	5.21	A	N
ATOM	379	C	LYS	A	579	26.666	69.087	4.726	1.00	5.05	A	C
ATOM	380	O	LYS	A	579	26.479	69.636	3.641	1.00	5.48	A	O
ATOM	381	N	ALA	A	580	25.829	69.176	5.752	1.00	4.48	A	N
ATOM	382	CA	ALA	A	580	24.603	69.934	5.704	1.00	4.02	A	C
ATOM	383	CB	ALA	A	580	23.587	69.300	6.624	1.00	4.94	A	C
ATOM	384	C	ALA	A	580	24.874	71.379	6.119	1.00	3.86	A	C
ATOM	385	O	ALA	A	580	23.955	72.194	6.168	1.00	5.24	A	O
ATOM	386	N	ILE	A	581	26.131	71.685	6.438	1.00	2.99	A	N
ATOM	387	CA	ILE	A	581	26.525	73.038	6.812	1.00	2.14	A	C
ATOM	388	CB	ILE	A	581	27.938	73.089	7.424	1.00	0.00	A	C
ATOM	389	CG2	ILE	A	581	28.110	74.365	8.194	1.00	0.00	A	C
ATOM	390	CG1	ILE	A	581	28.184	71.899	8.339	1.00	0.00	A	C
ATOM	391	CD1	ILE	A	581	27.228	71.800	9.482	1.00	0.00	A	C
ATOM	392	C	ILE	A	581	26.617	73.745	5.465	1.00	3.53	A	C
ATOM	393	O	ILE	A	581	27.157	73.172	4.509	1.00	3.17	A	O
ATOM	394	N	PRO	A	582	26.070	74.975	5.348	1.00	4.06	A	N
ATOM	395	CD	PRO	A	582	25.086	75.627	6.231	1.00	3.29	A	C
ATOM	396	CA	PRO	A	582	26.149	75.682	4.066	1.00	3.07	A	C
ATOM	397	CB	PRO	A	582	25.485	77.015	4.382	1.00	2.41	A	C
ATOM	398	CG	PRO	A	582	24.388	76.599	5.293	1.00	1.91	A	C
ATOM	399	C	PRO	A	582	27.589	75.838	3.562	1.00	3.62	A	C
ATOM	400	O	PRO	A	582	28.492	76.218	4.309	1.00	1.88	A	O
ATOM	401	N	GLY	A	583	27.797	75.514	2.293	1.00	3.11	A	N
ATOM	402	CA	GLY	A	583	29.122	75.643	1.718	1.00	4.87	A	C
ATOM	403	C	GLY	A	583	30.148	74.579	2.069	1.00	5.62	A	C
ATOM	404	O	GLY	A	583	31.265	74.616	1.550	1.00	5.44	A	O
ATOM	405	N	PHE	A	584	29.798	73.634	2.938	1.00	6.57	A	N
ATOM	406	CA	PHE	A	584	30.748	72.588	3.296	1.00	7.01	A	C
ATOM	407	CB	PHE	A	584	30.152	71.629	4.331	1.00	5.98	A	C
ATOM	408	CG	PHE	A	584	31.185	70.805	5.061	1.00	4.23	A	C
ATOM	409	CD1	PHE	A	584	31.961	71.369	6.073	1.00	3.98	A	C
ATOM	410	CD2	PHE	A	584	31.408	69.475	4.718	1.00	4.05	A	C
ATOM	411	CE1	PHE	A	584	32.948	70.616	6.731	1.00	3.51	A	C
ATOM	412	CE2	PHE	A	584	32.389	68.727	5.371	1.00	3.22	A	C
ATOM	413	CZ	PHE	A	584	33.159	69.299	6.376	1.00	2.80	A	C
ATOM	414	C	PHE	A	584	31.108	71.826	2.024	1.00	7.29	A	C
ATOM	415	O	PHE	A	584	32.280	71.729	1.669	1.00	8.14	A	O
ATOM	416	N	ARG	A	585	30.105	71.292	1.332	1.00	7.32	A	N
ATOM	417	CA	ARG	A	585	30.368	70.557	0.103	1.00	7.84	A	C
ATOM	418	CB	ARG	A	585	29.073	70.246	-0.654	1.00	10.41	A	C
ATOM	419	CG	ARG	A	585	29.308	69.747	-2.093	1.00	11.98	A	C
ATOM	420	CD	ARG	A	585	28.025	69.290	-2.781	1.00	12.55	A	C
ATOM	421	NE	ARG	A	585	28.190	69.164	-4.233	1.00	13.19	A	N
ATOM	422	CZ	ARG	A	585	27.188	68.961	-5.090	1.00	13.05	A	C
ATOM	423	NH1	ARG	A	585	25.938	68.854	-4.649	1.00	12.44	A	N
ATOM	424	NH2	ARG	A	585	27.431	68.891	-6.391	1.00	11.86	A	N
ATOM	425	C	ARG	A	585	31.267	71.384	-0.792	1.00	7.33	A	C
ATOM	426	O	ARG	A	585	32.071	70.853	-1.546	1.00	7.62	A	O
ATOM	427	N	ASN	A	586	31.126	72.696	-0.702	1.00	6.78	A	N
ATOM	428	CA	ASN	A	586	31.923	73.586	-1.524	1.00	6.33	A	C
ATOM	429	CB	ASN	A	586	31.558	75.044	-1.232	1.00	6.55	A	C
ATOM	430	CG	ASN	A	586	30.123	75.374	-1.615	1.00	6.08	A	C
ATOM	431	OD1	ASN	A	586	29.176	74.808	-1.072	1.00	6.71	A	O
ATOM	432	ND2	ASN	A	586	29.961	76.292	-2.557	1.00	6.45	A	N
ATOM	433	C	ASN	A	586	33.401	73.343	-1.280	1.00	5.95	A	C
ATOM	434	O	ASN	A	586	34.225	73.507	-2.183	1.00	6.08	A	O
ATOM	435	N	LEU	A	587	33.730	72.932	-0.061	1.00	4.83	A	N
ATOM	436	CA	LEU	A	587	35.114	72.664	0.291	1.00	4.49	A	C
ATOM	437	CB	LEU	A	587	35.320	72.728	1.810	1.00	1.95	A	C
ATOM	438	CG	LEU	A	587	35.096	74.062	2.526	1.00	0.00	A	C
ATOM	439	CD1	LEU	A	587	35.711	74.010	3.912	1.00	0.00	A	C
ATOM	440	CD2	LEU	A	587	35.711	75.183	1.720	1.00	0.00	A	C
ATOM	441	C	LEU	A	587	35.594	71.314	-0.227	1.00	6.08	A	C
ATOM	442	O	LEU	A	587	34.973	70.278	0.014	1.00	5.03	A	O
ATOM	443	N	HIS	A	588	36.706	71.363	-0.954	1.00	7.97	A	N
ATOM	444	CA	HIS	A	588	37.375	70.200	-1.528	1.00	7.66	A	C
ATOM	445	CB	HIS	A	588	38.853	70.556	-1.721	1.00	8.59	A	C
ATOM	446	CG	HIS	A	588	39.549	69.792	-2.803	1.00	10.62	A	C
ATOM	447	CD2	HIS	A	588	39.101	68.861	-3.675	1.00	11.30	A	C
ATOM	448	ND1	HIS	A	588	40.887	69.971	-3.086	1.00	11.32	A	N

ATOM	449	CE1	HIS	A	588	41.234	69.183	-4.086	1.00	11.35	A	C
ATOM	450	NE2	HIS	A	588	40.169	68.498	-4.461	1.00	11.77	A	N
ATOM	451	C	HIS	A	588	37.228	69.062	-0.514	1.00	6.17	A	C
ATOM	452	O	HIS	A	588	37.194	69.313	0.696	1.00	7.07	A	O
ATOM	453	N	LEU	A	589	37.137	67.822	-0.987	1.00	3.08	A	N
ATOM	454	CA	LEU	A	589	36.980	66.710	-0.065	1.00	1.54	A	C
ATOM	455	CB	LEU	A	589	36.664	65.423	-0.824	1.00	1.60	A	C
ATOM	456	CG	LEU	A	589	35.194	65.169	-1.189	1.00	1.11	A	C
ATOM	457	CD1	LEU	A	589	34.796	65.925	-2.457	1.00	0.21	A	C
ATOM	458	CD2	LEU	A	589	35.005	63.680	-1.404	1.00	0.60	A	C
ATOM	459	C	LEU	A	589	38.206	66.516	0.829	1.00	1.42	A	O
ATOM	460	O	LEU	A	589	38.089	66.040	1.967	1.00	1.35	A	N
ATOM	461	N	ASP	A	590	39.384	66.876	0.328	1.00	1.96	A	C
ATOM	462	CA	ASP	A	590	40.576	66.741	1.145	1.00	3.02	A	C
ATOM	463	CB	ASP	A	590	41.808	67.220	0.403	1.00	2.72	A	C
ATOM	464	CG	ASP	A	590	42.280	66.228	-0.619	1.00	4.98	A	O
ATOM	465	OD1	ASP	A	590	41.535	65.958	-1.588	1.00	5.51	A	O
ATOM	466	OD2	ASP	A	590	43.401	65.704	-0.446	1.00	7.12	A	C
ATOM	467	C	ASP	A	590	40.331	67.622	2.338	1.00	3.28	A	O
ATOM	468	O	ASP	A	590	40.728	67.297	3.451	1.00	1.93	A	N
ATOM	469	N	ASP	A	591	39.646	68.735	2.087	1.00	4.09	A	C
ATOM	470	CA	ASP	A	591	39.320	69.702	3.122	1.00	3.32	A	C
ATOM	471	CB	ASP	A	591	38.713	70.968	2.515	1.00	2.03	A	C
ATOM	472	CG	ASP	A	591	39.606	71.602	1.456	1.00	2.28	A	O
ATOM	473	OD1	ASP	A	591	40.845	71.444	1.533	1.00	1.79	A	O
ATOM	474	OD2	ASP	A	591	39.067	72.275	0.547	1.00	2.67	A	C
ATOM	475	C	ASP	A	591	38.339	69.085	4.081	1.00	3.14	A	O
ATOM	476	O	ASP	A	591	38.677	68.816	5.231	1.00	3.40	A	N
ATOM	477	N	GLN	A	592	37.126	68.858	3.589	1.00	2.76	A	C
ATOM	478	CA	GLN	A	592	36.045	68.257	4.372	1.00	3.71	A	C
ATOM	479	CB	GLN	A	592	34.986	67.668	3.435	1.00	4.09	A	C
ATOM	480	CG	GLN	A	592	34.359	68.665	2.464	1.00	2.57	A	C
ATOM	481	CD	GLN	A	592	33.220	68.065	1.659	1.00	1.45	A	O
ATOM	482	OE1	GLN	A	592	32.171	67.712	2.202	1.00	0.57	A	N
ATOM	483	NE2	GLN	A	592	33.425	67.947	0.355	1.00	1.06	A	C
ATOM	484	C	GLN	A	592	36.547	67.154	5.306	1.00	4.37	A	O
ATOM	485	O	GLN	A	592	36.344	67.202	6.525	1.00	4.05	A	N
ATOM	486	N	MET	A	593	37.197	66.152	4.723	1.00	4.47	A	C
ATOM	487	CA	MET	A	593	37.727	65.062	5.514	1.00	3.67	A	C
ATOM	488	CB	MET	A	593	38.413	64.042	4.614	1.00	3.57	A	C
ATOM	489	CG	MET	A	593	37.455	63.290	3.693	1.00	4.07	A	S
ATOM	490	SD	MET	A	593	36.208	62.250	4.528	1.00	4.62	A	C
ATOM	491	CE	MET	A	593	35.748	61.193	3.146	1.00	2.82	A	C
ATOM	492	C	MET	A	593	38.704	65.605	6.539	1.00	2.45	A	O
ATOM	493	O	MET	A	593	38.622	65.265	7.706	1.00	2.80	A	N
ATOM	494	N	THR	A	594	39.620	66.462	6.108	1.00	1.88	A	C
ATOM	495	CA	THR	A	594	40.599	67.043	7.026	1.00	2.57	A	C
ATOM	496	CB	THR	A	594	41.516	68.101	6.314	1.00	5.68	A	O
ATOM	497	OG1	THR	A	594	42.405	67.439	5.402	1.00	6.99	A	C
ATOM	498	CG2	THR	A	594	42.347	68.887	7.338	1.00	6.06	A	C
ATOM	499	C	THR	A	594	39.910	67.725	8.202	1.00	0.49	A	O
ATOM	500	O	THR	A	594	40.265	67.509	9.361	1.00	0.00	A	N
ATOM	501	N	LEU	A	595	38.915	68.544	7.899	1.00	0.00	A	C
ATOM	502	CA	LEU	A	595	38.219	69.265	8.941	1.00	0.00	A	C
ATOM	503	CB	LEU	A	595	37.563	70.499	8.364	1.00	0.00	A	C
ATOM	504	CG	LEU	A	595	38.591	71.557	8.015	1.00	0.00	A	C
ATOM	505	CD1	LEU	A	595	37.952	72.555	7.083	1.00	0.00	A	C
ATOM	506	CD2	LEU	A	595	39.107	72.210	9.282	1.00	0.00	A	C
ATOM	507	C	LEU	A	595	37.203	68.453	9.683	1.00	0.00	A	O
ATOM	508	O	LEU	A	595	36.651	68.917	10.677	1.00	0.00	A	N
ATOM	509	N	LEU	A	596	36.938	67.245	9.210	1.00	0.00	A	C
ATOM	510	CA	LEU	A	596	35.983	66.417	9.913	1.00	0.00	A	C
ATOM	511	CB	LEU	A	596	35.085	65.662	8.939	1.00	0.00	A	C
ATOM	512	CG	LEU	A	596	33.615	66.017	9.167	1.00	0.00	A	C
ATOM	513	CD1	LEU	A	596	32.773	65.430	8.087	1.00	0.00	A	C
ATOM	514	CD2	LEU	A	596	33.172	65.525	10.513	1.00	0.00	A	C
ATOM	515	C	LEU	A	596	36.690	65.460	10.845	1.00	0.00	A	O
ATOM	516	O	LEU	A	596	36.050	64.868	11.706	1.00	0.00	A	N
ATOM	517	N	GLN	A	597	38.009	65.327	10.673	1.00	0.00	A	C
ATOM	518	CA	GLN	A	597	38.846	64.452	11.510	1.00	0.00	A	C
ATOM	519	CB	GLN	A	597	40.095	63.946	10.758	1.00	0.00	A	C
ATOM	520	CG	GLN	A	597	39.904	63.337	9.374	1.00	0.00	A	C
ATOM	521	CD	GLN	A	597	41.230	62.902	8.731	1.00	0.00	A	O
ATOM	522	OE1	GLN	A	597	41.330	62.779	7.522	1.00	0.00	A	N
ATOM	523	NE2	GLN	A	597	42.242	62.660	9.551	1.00	0.00	A	C
ATOM	524	C	GLN	A	597	39.336	65.261	12.716	1.00	1.04	A	O
ATOM	525	O	GLN	A	597	39.773	64.692	13.718	1.00	0.81	A	N
ATOM	526	N	TYR	A	598	39.278	66.590	12.593	1.00	1.70	A	C
ATOM	527	CA	TYR	A	598	39.717	67.508	13.645	1.00	1.57	A	C
ATOM	528	CB	TYR	A	598	40.278	68.798	13.045	1.00	0.46	A	C
ATOM	529	CG	TYR	A	598	41.656	68.679	12.476	1.00	0.00	A	C

ATOM	530	CD1	TYR	A	598	42.696	68.161	13.235	1.00	0.00	A	C
ATOM	531	CE1	TYR	A	598	43.963	68.039	12.717	1.00	0.69	A	C
ATOM	532	CD2	TYR	A	598	41.920	69.077	11.182	1.00	0.00	A	C
ATOM	533	CE2	TYR	A	598	43.186	68.961	10.647	1.00	0.00	A	C
ATOM	534	CZ	TYR	A	598	44.203	68.439	11.420	1.00	0.91	A	C
ATOM	535	OH	TYR	A	598	45.458	68.305	10.887	1.00	2.35	A	O
ATOM	536	C	TYR	A	598	38.606	67.896	14.595	1.00	1.97	A	C
ATOM	537	O	TYR	A	598	38.842	68.101	15.772	1.00	2.93	A	O
ATOM	538	N	SER	A	599	37.393	68.011	14.080	1.00	2.26	A	N
ATOM	539	CA	SER	A	599	36.270	68.400	14.910	1.00	4.13	A	C
ATOM	540	CB	SER	A	599	35.386	69.379	14.132	1.00	6.03	A	C
ATOM	541	OG	SER	A	599	35.217	68.979	12.783	1.00	5.27	A	O
ATOM	542	C	SER	A	599	35.407	67.274	15.478	1.00	5.52	A	C
ATOM	543	O	SER	A	599	34.331	67.537	16.013	1.00	8.08	A	O
ATOM	544	N	TRP	A	600	35.845	66.024	15.400	1.00	6.06	A	N
ATOM	545	CA	TRP	A	600	34.967	65.006	15.936	1.00	6.37	A	C
ATOM	546	CB	TRP	A	600	35.376	63.577	15.487	1.00	9.43	A	C
ATOM	547	CG	TRP	A	600	36.557	62.934	16.122	1.00	9.07	A	C
ATOM	548	CD2	TRP	A	600	36.535	61.867	17.086	1.00	10.85	A	C
ATOM	549	CE2	TRP	A	600	37.880	61.559	17.401	1.00	10.00	A	C
ATOM	550	CE3	TRP	A	600	35.510	61.145	17.715	1.00	9.96	A	C
ATOM	551	CD1	TRP	A	600	37.872	63.217	15.894	1.00	9.72	A	C
ATOM	552	NE1	TRP	A	600	38.674	62.394	16.660	1.00	10.68	A	N
ATOM	553	C22	TRP	A	600	38.226	60.557	18.318	1.00	8.99	A	C
ATOM	554	C23	TRP	A	600	35.858	60.145	18.629	1.00	9.07	A	C
ATOM	555	CH2	TRP	A	600	37.207	59.867	18.920	1.00	9.32	A	C
ATOM	556	C	TRP	A	600	34.796	65.139	17.448	1.00	5.65	A	O
ATOM	557	O	TRP	A	600	33.757	65.610	17.901	1.00	6.26	A	N
ATOM	558	N	MET	A	601	35.796	64.776	18.234	1.00	2.98	A	C
ATOM	559	CA	MET	A	601	35.644	64.893	19.673	1.00	0.39	A	C
ATOM	560	CB	MET	A	601	36.966	64.542	20.372	1.00	0.50	A	C
ATOM	561	CG	MET	A	601	36.920	64.495	21.900	1.00	0.00	A	S
ATOM	562	SD	MET	A	601	35.592	63.524	22.601	1.00	0.00	A	C
ATOM	563	CE	MET	A	601	36.310	62.772	24.011	1.00	0.00	A	C
ATOM	564	C	MET	A	601	35.165	66.301	20.041	1.00	0.00	A	O
ATOM	565	O	MET	A	601	34.652	66.516	21.123	1.00	0.00	A	N
ATOM	566	N	PHE	A	602	35.307	67.267	19.144	1.00	0.00	A	C
ATOM	567	CA	PHE	A	602	34.847	68.625	19.457	1.00	0.37	A	C
ATOM	568	CB	PHE	A	602	35.403	69.654	18.460	1.00	1.81	A	C
ATOM	569	CG	PHE	A	602	36.871	69.930	18.633	1.00	1.20	A	C
ATOM	570	CD1	PHE	A	602	37.704	70.039	17.530	1.00	0.00	A	C
ATOM	571	CD2	PHE	A	602	37.426	70.032	19.902	1.00	0.57	A	C
ATOM	572	CE1	PHE	A	602	39.066	70.234	17.689	1.00	0.23	A	C
ATOM	573	CE2	PHE	A	602	38.791	70.229	20.069	1.00	1.00	A	C
ATOM	574	CZ	PHE	A	602	39.612	70.327	18.962	1.00	0.83	A	C
ATOM	575	C	PHE	A	602	33.330	68.658	19.437	1.00	1.06	A	O
ATOM	576	O	PHE	A	602	32.707	69.036	20.427	1.00	1.08	A	N
ATOM	577	N	LEU	A	603	32.739	68.277	18.307	1.00	2.03	A	C
ATOM	578	CA	LEU	A	603	31.288	68.227	18.207	1.00	3.01	A	C
ATOM	579	CB	LEU	A	603	30.865	67.720	16.832	1.00	3.77	A	C
ATOM	580	CG	LEU	A	603	31.033	68.729	15.701	1.00	5.04	A	C
ATOM	581	CD1	LEU	A	603	30.857	68.044	14.362	1.00	4.29	A	C
ATOM	582	CD2	LEU	A	603	30.026	69.841	15.869	1.00	5.20	A	C
ATOM	583	C	LEU	A	603	30.816	67.258	19.299	1.00	2.59	A	C
ATOM	584	O	LEU	A	603	30.085	67.643	20.211	1.00	4.55	A	O
ATOM	585	N	MET	A	604	31.256	66.006	19.210	1.00	0.05	A	N
ATOM	586	CA	MET	A	604	30.914	64.992	20.193	1.00	0.00	A	C
ATOM	587	CB	MET	A	604	31.958	63.884	20.163	1.00	0.00	A	C
ATOM	588	CG	MET	A	604	32.042	63.176	18.833	1.00	0.00	A	S
ATOM	589	SD	MET	A	604	30.526	62.285	18.507	1.00	0.00	A	C
ATOM	590	CE	MET	A	604	31.103	60.590	18.449	1.00	0.00	A	C
ATOM	591	C	MET	A	604	30.873	65.619	21.580	1.00	0.00	A	O
ATOM	592	O	MET	A	604	29.800	65.868	22.122	1.00	0.00	A	N
ATOM	593	N	ALA	A	605	32.052	65.888	22.136	1.00	0.00	A	C
ATOM	594	CA	ALA	A	605	32.198	66.487	23.467	1.00	0.00	A	C
ATOM	595	CB	ALA	A	605	33.655	66.856	23.717	1.00	0.00	A	C
ATOM	596	C	ALA	A	605	31.323	67.705	23.704	1.00	0.00	A	O
ATOM	597	O	ALA	A	605	30.943	67.991	24.835	1.00	0.00	A	N
ATOM	598	N	PHE	A	606	31.005	68.435	22.648	1.00	0.00	A	C
ATOM	599	CA	PHE	A	606	30.172	69.606	22.814	1.00	0.00	A	C
ATOM	600	CB	PHE	A	606	30.349	70.556	21.4632	1.00	0.00	A	C
ATOM	601	CG	PHE	A	606	29.873	71.962	21.908	1.00	0.00	A	C
ATOM	602	CD1	PHE	A	606	30.380	72.677	22.978	1.00	0.00	A	C
ATOM	603	CD2	PHE	A	606	28.907	72.553	21.108	1.00	0.00	A	C
ATOM	604	CE1	PHE	A	606	29.937	73.932	23.241	1.00	0.00	A	C
ATOM	605	CE2	PHE	A	606	28.462	73.810	21.369	1.00	0.00	A	C
ATOM	606	CZ	PHE	A	606	28.973	74.504	22.436	1.00	0.00	A	C
ATOM	607	C	PHE	A	606	28.729	69.172	22.930	1.00	0.00	A	O
ATOM	608	O	PHE	A	606	28.099	69.381	23.955	1.00	0.00	A	N
ATOM	609	N	ALA	A	607	28.226	68.557	21.867	1.00	0.00	A	C
ATOM	610	CA	ALA	A	607	26.860	68.056	21.804	1.00	0.49	A	C

ATOM	611	CB	ALA	A	607	26.797	66.848	20.888	1.00	0.14	A	C
ATOM	612	C	ALA	A	607	26.392	67.671	23.189	1.00	1.53	A	C
ATOM	613	O	ALA	A	607	25.392	68.178	23.695	1.00	2.78	A	O
ATOM	614	N	LEU	A	608	27.126	66.763	23.804	1.00	1.69	A	N
ATOM	615	CA	LEU	A	608	26.786	66.322	25.139	1.00	2.07	A	C
ATOM	616	CB	LEU	A	608	27.871	65.386	25.663	1.00	2.30	A	C
ATOM	617	CG	LEU	A	608	27.537	64.643	26.947	1.00	1.86	A	C
ATOM	618	CD1	LEU	A	608	26.366	63.743	26.694	1.00	2.95	A	C
ATOM	619	CD2	LEU	A	608	28.720	63.839	27.395	1.00	2.57	A	C
ATOM	620	C	LEU	A	608	26.652	67.530	26.064	1.00	2.18	A	C
ATOM	621	O	LEU	A	608	25.592	67.756	26.644	1.00	1.10	A	O
ATOM	622	N	GLY	A	609	27.734	68.301	26.185	1.00	2.31	A	N
ATOM	623	CA	GLY	A	609	27.745	69.475	27.041	1.00	0.69	A	C
ATOM	624	C	GLY	A	609	26.392	70.154	27.105	1.00	0.00	A	C
ATOM	625	O	GLY	A	609	25.890	70.475	28.183	1.00	0.06	A	O
ATOM	626	N	TRP	A	610	25.798	70.361	25.939	1.00	0.00	A	N
ATOM	627	CA	TRP	A	610	24.495	70.993	25.845	1.00	0.00	A	C
ATOM	628	CB	TRP	A	610	24.262	71.459	24.404	1.00	0.79	A	C
ATOM	629	CG	TRP	A	610	22.866	71.864	24.090	1.00	1.59	A	C
ATOM	630	CD2	TRP	A	610	22.338	73.191	24.100	1.00	0.93	A	C
ATOM	631	CE2	TRP	A	610	20.958	73.095	23.814	1.00	1.43	A	C
ATOM	632	CE3	TRP	A	610	22.893	74.454	24.331	1.00	1.29	A	C
ATOM	633	CD1	TRP	A	610	21.821	71.038	23.799	1.00	2.70	A	C
ATOM	634	NE1	TRP	A	610	20.668	71.770	23.632	1.00	2.17	A	N
ATOM	635	CZ2	TRP	A	610	20.125	74.211	23.757	1.00	1.17	A	C
ATOM	636	CZ3	TRP	A	610	22.062	75.564	24.274	1.00	1.18	A	C
ATOM	637	CH2	TRP	A	610	20.693	75.432	23.989	1.00	0.51	A	C
ATOM	638	C	TRP	A	610	23.404	70.025	26.299	1.00	0.00	A	C
ATOM	639	O	TRP	A	610	22.701	70.306	27.270	1.00	0.00	A	O
ATOM	640	N	ARG	A	611	23.277	68.886	25.614	1.00	0.00	A	N
ATOM	641	CA	ARG	A	611	22.265	67.887	25.968	1.00	0.00	A	C
ATOM	642	CB	ARG	A	611	22.646	66.493	25.467	1.00	0.00	A	C
ATOM	643	CG	ARG	A	611	22.941	66.368	23.989	1.00	0.00	A	C
ATOM	644	CD	ARG	A	611	23.344	64.937	23.646	1.00	0.00	A	C
ATOM	645	NE	ARG	A	611	24.021	64.858	22.360	1.00	0.00	A	N
ATOM	646	CZ	ARG	A	611	23.522	65.330	21.220	1.00	0.00	A	C
ATOM	647	NH1	ARG	A	611	22.338	65.917	21.204	1.00	0.00	A	N
ATOM	648	NH2	ARG	A	611	24.208	65.218	20.090	1.00	0.00	A	N
ATOM	649	C	ARG	A	611	22.093	67.807	27.475	1.00	0.00	A	C
ATOM	650	O	ARG	A	611	20.992	67.966	27.980	1.00	0.00	A	O
ATOM	651	N	SER	A	612	23.188	67.560	28.190	1.00	0.67	A	N
ATOM	652	CA	SER	A	612	23.138	67.452	29.648	1.00	1.96	A	C
ATOM	653	CB	SER	A	612	24.209	66.498	30.177	1.00	2.19	A	C
ATOM	654	OG	SER	A	612	25.486	67.100	30.200	1.00	4.26	A	O
ATOM	655	C	SER	A	612	23.317	68.799	30.313	1.00	2.61	A	C
ATOM	656	O	SER	A	612	24.264	69.015	31.058	1.00	1.54	A	O
ATOM	657	N	TYR	A	613	22.384	69.695	30.026	1.00	3.78	A	N
ATOM	658	CA	TYR	A	613	22.359	71.045	30.569	1.00	4.65	A	C
ATOM	659	CB	TYR	A	613	23.526	71.869	30.020	1.00	5.98	A	C
ATOM	660	CG	TYR	A	613	23.181	73.317	29.797	1.00	5.30	A	C
ATOM	661	CD1	TYR	A	613	23.098	74.212	30.858	1.00	6.21	A	C
ATOM	662	CE1	TYR	A	613	22.688	75.528	30.658	1.00	5.08	A	C
ATOM	663	CD2	TYR	A	613	22.852	73.771	28.528	1.00	6.15	A	C
ATOM	664	CE2	TYR	A	613	22.441	75.076	28.315	1.00	6.69	A	C
ATOM	665	CZ	TYR	A	613	22.358	75.948	29.381	1.00	5.38	A	C
ATOM	666	OH	TYR	A	613	21.922	77.223	29.150	1.00	4.66	A	O
ATOM	667	C	TYR	A	613	21.037	71.613	30.098	1.00	5.06	A	C
ATOM	668	O	TYR	A	613	20.662	72.731	30.429	1.00	5.38	A	O
ATOM	669	N	ARG	A	614	20.343	70.812	29.302	1.00	5.49	A	N
ATOM	670	CA	ARG	A	614	19.044	71.171	28.772	1.00	5.93	A	C
ATOM	671	CB	ARG	A	614	19.095	71.260	27.239	1.00	5.63	A	C
ATOM	672	CG	ARG	A	614	17.795	71.735	26.580	1.00	5.65	A	C
ATOM	673	CD	ARG	A	614	17.943	71.986	25.069	1.00	5.28	A	C
ATOM	674	NE	ARG	A	614	16.656	72.264	24.427	1.00	4.84	A	N
ATOM	675	CZ	ARG	A	614	16.497	72.543	23.136	1.00	3.40	A	C
ATOM	676	NH1	ARG	A	614	17.545	72.584	22.333	1.00	3.79	A	N
ATOM	677	NH2	ARG	A	614	15.289	72.784	22.650	1.00	1.72	A	N
ATOM	678	G	ARG	A	614	18.068	70.081	29.205	1.00	6.00	A	C
ATOM	679	O	ARG	A	614	16.976	70.385	29.683	1.00	7.53	A	O
ATOM	680	N	GLN	A	615	18.484	68.817	29.069	1.00	5.01	A	N
ATOM	681	CA	GLN	A	615	17.636	67.673	29.410	1.00	4.72	A	C
ATOM	682	CB	GLN	A	615	17.659	66.636	28.281	1.00	6.29	A	C
ATOM	683	CG	GLN	A	615	16.278	66.340	27.689	1.00	10.07	A	C
ATOM	684	CD	GLN	A	615	15.322	65.653	28.678	1.00	11.83	A	C
ATOM	685	OE1	GLN	A	615	14.090	65.699	28.515	1.00	11.71	A	O
ATOM	686	NE2	GLN	A	615	15.888	65.005	29.699	1.00	13.29	A	N
ATOM	687	C	GLN	A	615	17.935	66.968	30.716	1.00	4.69	A	C
ATOM	688	O	GLN	A	615	17.879	65.742	30.779	1.00	1.68	A	O
ATOM	689	N	SER	A	616	18.241	67.742	31.753	1.00	6.09	A	N
ATOM	690	CA	SER	A	616	18.525	67.193	33.083	1.00	6.97	A	C
ATOM	691	CB	SER	A	616	19.489	65.997	32.991	1.00	5.88	A	C



ATOM	773	C	LEU	A	627	21.849	58.173	30.090	1.00	1.52	A	C
ATOM	774	O	LEU	A	627	21.968	59.179	29.406	1.00	0.77	A	O
ATOM	775	N	ILE	A	628	22.044	58.189	31.396	1.00	1.10	A	N
ATOM	776	CA	ILE	A	628	22.404	59.430	32.055	1.00	0.29	A	C
ATOM	777	CB	ILE	A	628	21.163	60.202	32.540	1.00	0.57	A	C
ATOM	778	CG2	ILE	A	628	21.445	61.678	32.528	1.00	0.00	A	C
ATOM	779	CG1	ILE	A	628	19.952	59.884	31.676	1.00	0.62	A	C
ATOM	780	CD1	ILE	A	628	19.284	58.556	32.018	1.00	1.08	A	C
ATOM	781	C	ILE	A	628	23.253	59.141	33.279	1.00	0.46	A	C
ATOM	782	O	ILE	A	628	22.722	59.017	34.380	1.00	1.45	A	O
ATOM	783	N	ILE	A	629	24.562	59.026	33.118	1.00	0.11	A	N
ATOM	784	CA	ILE	A	629	25.362	58.747	34.289	1.00	2.20	A	C
ATOM	785	CB	ILE	A	629	26.852	58.775	33.964	1.00	3.14	A	C
ATOM	786	CG2	ILE	A	629	27.682	58.511	35.231	1.00	1.51	A	C
ATOM	787	CG1	ILE	A	629	27.146	57.703	32.916	1.00	2.96	A	C
ATOM	788	CD1	ILE	A	629	28.611	57.493	32.664	1.00	3.69	A	C
ATOM	789	C	ILE	A	629	25.032	59.762	35.374	1.00	3.38	A	C
ATOM	790	O	ILE	A	629	25.378	60.930	35.264	1.00	4.88	A	O
ATOM	791	N	ASN	A	630	24.337	59.295	36.408	1.00	4.33	A	N
ATOM	792	CA	ASN	A	630	23.908	60.108	37.551	1.00	4.29	A	C
ATOM	793	CB	ASN	A	630	23.217	59.200	38.574	1.00	3.81	A	C
ATOM	794	CG	ASN	A	630	22.363	58.119	37.915	1.00	4.39	A	C
ATOM	795	OD1	ASN	A	630	22.838	57.371	37.052	1.00	3.09	A	O
ATOM	796	ND2	ASN	A	630	21.098	58.028	38.325	1.00	4.13	A	N
ATOM	797	C	ASN	A	630	25.080	60.827	38.212	1.00	4.98	A	C
ATOM	798	O	ASN	A	630	25.912	61.415	37.539	1.00	4.16	A	O
ATOM	799	N	GLU	A	631	25.137	60.798	39.537	1.00	6.52	A	N
ATOM	800	CA	GLU	A	631	26.249	61.431	40.236	1.00	8.03	A	C
ATOM	801	CB	GLU	A	631	25.801	62.635	41.079	1.00	9.15	A	C
ATOM	802	CG	GLU	A	631	27.006	63.424	41.649	1.00	10.50	A	C
ATOM	803	CD	GLU	A	631	26.635	64.510	42.660	1.00	11.16	A	C
ATOM	804	OE1	GLU	A	631	26.047	64.183	43.719	1.00	11.47	A	O
ATOM	805	OE2	GLU	A	631	26.950	65.692	42.388	1.00	10.90	A	O
ATOM	806	C	GLU	A	631	26.979	60.446	41.135	1.00	8.01	A	C
ATOM	807	O	GLU	A	631	28.205	60.376	41.108	1.00	8.95	A	O
ATOM	808	N	GLN	A	632	26.239	59.693	41.943	1.00	7.43	A	N
ATOM	809	CA	GLN	A	632	26.882	58.724	42.816	1.00	7.50	A	C
ATOM	810	CB	GLN	A	632	25.907	58.234	43.899	1.00	7.13	A	C
ATOM	811	CG	GLN	A	632	25.603	59.299	44.951	1.00	5.53	A	C
ATOM	812	CD	GLN	A	632	25.111	58.729	46.271	1.00	4.58	A	C
ATOM	813	OR1	GLN	A	632	25.721	58.945	47.324	1.00	2.81	A	O
ATOM	814	NE2	GLN	A	632	23.998	58.001	46.223	1.00	3.30	A	N
ATOM	815	C	GLN	A	632	27.427	57.554	41.987	1.00	8.43	A	C
ATOM	816	O	GLN	A	632	27.807	56.508	42.521	1.00	8.94	A	O
ATOM	817	N	ARG	A	633	27.476	57.764	40.676	1.00	8.83	A	N
ATOM	818	CA	ARG	A	633	27.974	56.780	39.727	1.00	9.35	A	C
ATOM	819	CB	ARG	A	633	26.881	56.470	38.703	1.00	9.45	A	C
ATOM	820	CG	ARG	A	633	27.223	55.430	37.632	1.00	10.20	A	C
ATOM	821	CD	ARG	A	633	27.180	54.000	38.178	1.00	11.55	A	C
ATOM	822	NE	ARG	A	633	26.059	53.756	39.100	1.00	12.60	A	N
ATOM	823	CZ	ARG	A	633	24.771	53.709	38.762	1.00	13.07	A	C
ATOM	824	NH1	ARG	A	633	24.388	53.883	37.503	1.00	14.00	A	N
ATOM	825	NH2	ARG	A	633	23.861	53.494	39.699	1.00	12.82	A	N
ATOM	826	C	ARG	A	633	29.198	57.369	39.019	1.00	9.65	A	C
ATOM	827	O	ARG	A	633	29.780	56.726	38.148	1.00	10.22	A	O
ATOM	828	N	MET	A	634	29.579	58.587	39.415	1.00	9.90	A	N
ATOM	829	CA	MET	A	634	30.711	59.323	38.831	1.00	9.96	A	C
ATOM	830	CB	MET	A	634	30.390	60.815	38.771	1.00	10.24	A	C
ATOM	831	CG	MET	A	634	28.977	61.126	38.305	1.00	13.69	A	C
ATOM	832	SD	MET	A	634	28.439	62.809	38.723	1.00	14.95	A	S
ATOM	833	CE	MET	A	634	28.956	63.686	37.228	1.00	14.68	A	C
ATOM	834	C	MET	A	634	32.006	59.154	39.614	1.00	9.16	A	C
ATOM	835	O	MET	A	634	32.723	60.133	39.852	1.00	8.99	A	O
ATOM	836	N	THR	A	635	32.294	57.914	40.010	1.00	7.65	A	N
ATOM	837	CA	THR	A	635	33.503	57.579	40.765	1.00	6.98	A	C
ATOM	838	CB	THR	A	635	33.231	57.431	42.249	1.00	8.59	A	C
ATOM	839	OG1	THR	A	635	32.469	56.231	42.463	1.00	7.94	A	O
ATOM	840	CG2	THR	A	635	32.472	58.663	42.783	1.00	9.13	A	C
ATOM	841	C	THR	A	635	33.934	56.221	40.298	1.00	6.09	A	C
ATOM	842	O	THR	A	635	35.116	55.883	40.292	1.00	5.31	A	O
ATOM	843	N	LEU	A	636	32.928	55.439	39.932	1.00	6.76	A	N
ATOM	844	CA	LEU	A	636	33.123	54.091	39.435	1.00	6.94	A	C
ATOM	845	CB	LEU	A	636	31.783	53.361	39.326	1.00	5.62	A	C
ATOM	846	CG	LEU	A	636	31.739	51.948	39.904	1.00	4.04	A	C
ATOM	847	CD1	LEU	A	636	30.455	51.281	39.487	1.00	3.26	A	C
ATOM	848	CD2	LEU	A	636	32.911	51.137	39.405	1.00	4.29	A	C
ATOM	849	C	LEU	A	636	33.796	54.129	38.068	1.00	8.21	A	C
ATOM	850	O	LEU	A	636	34.474	53.178	37.697	1.00	8.27	A	O
ATOM	851	N	PRO	A	637	33.620	55.220	37.290	1.00	9.08	A	N
ATOM	852	CD	PRO	A	637	33.003	56.548	37.459	1.00	8.92	A	C
ATOM	853	CA	PRO	A	637	34.309	55.155	36.005	1.00	10.63	A	C

ATOM	854	CB	PRO	A	637	33.925	56.478	35.341	1.00	9.77	A	C
ATOM	855	CG	PRO	A	637	33.784	57.385	36.478	1.00	8.43	A	C
ATOM	856	C	PRO	A	637	35.803	55.029	36.246	1.00	12.24	A	C
ATOM	857	O	PRO	A	637	36.318	55.515	37.252	1.00	14.00	A	O
ATOM	858	N	ASP	A	638	36.498	54.345	35.346	1.00	12.76	A	N
ATOM	859	CA	ASP	A	638	37.936	54.211	35.494	1.00	12.16	A	C
ATOM	860	CB	ASP	A	638	38.520	53.282	34.426	1.00	11.16	A	C
ATOM	861	CG	ASP	A	638	39.918	52.810	34.773	1.00	9.06	A	C
ATOM	862	OD1	ASP	A	638	40.630	53.555	35.483	1.00	6.47	A	O
ATOM	863	OD2	ASP	A	638	40.303	51.701	34.331	1.00	7.55	A	O
ATOM	864	C	ASP	A	638	38.450	55.634	35.282	1.00	13.37	A	C
ATOM	865	O	ASP	A	638	39.659	55.901	35.336	1.00	16.44	A	O
ATOM	866	N	MET	A	639	37.513	56.542	35.017	1.00	12.95	A	N
ATOM	867	CA	MET	A	639	37.862	57.931	34.821	1.00	12.79	A	C
ATOM	868	CB	MET	A	639	38.131	58.234	33.334	1.00	13.62	A	C
ATOM	869	CG	MET	A	639	36.930	58.328	32.412	1.00	9.98	A	C
ATOM	870	SD	MET	A	639	37.433	59.097	30.859	1.00	7.83	A	S
ATOM	871	CE	MET	A	639	37.900	57.616	29.885	1.00	5.47	A	C
ATOM	872	C	MET	A	639	36.863	58.931	35.396	1.00	13.49	A	C
ATOM	873	O	MET	A	639	36.098	59.583	34.672	1.00	12.33	A	O
ATOM	874	N	TYR	A	640	36.857	59.014	36.721	1.00	13.18	A	N
ATOM	875	CA	TYR	A	640	36.033	59.986	37.409	1.00	10.90	A	C
ATOM	876	CB	TYR	A	640	35.784	59.567	38.845	1.00	7.90	A	C
ATOM	877	CG	TYR	A	640	35.960	60.714	39.789	1.00	8.65	A	C
ATOM	878	CD1	TYR	A	640	34.971	61.692	39.924	1.00	9.47	A	C
ATOM	879	CE1	TYR	A	640	35.174	62.813	40.733	1.00	10.07	A	C
ATOM	880	CD2	TYR	A	640	37.157	60.881	40.491	1.00	9.70	A	C
ATOM	881	CE2	TYR	A	640	37.366	61.996	41.301	1.00	9.93	A	C
ATOM	882	CZ	TYR	A	640	36.373	62.953	41.414	1.00	9.95	A	C
ATOM	883	OH	TYR	A	640	36.585	64.051	42.204	1.00	11.59	A	O
ATOM	884	C	TYR	A	640	37.041	61.127	37.359	1.00	9.98	A	C
ATOM	885	O	TYR	A	640	36.714	62.309	37.445	1.00	8.68	A	O
ATOM	886	N	ASP	A	641	38.297	60.727	37.216	1.00	9.69	A	N
ATOM	887	CA	ASP	A	641	39.396	61.658	37.095	1.00	10.40	A	C
ATOM	888	CB	ASP	A	641	40.723	60.942	37.375	1.00	9.65	A	C
ATOM	889	CG	ASP	A	641	40.655	59.435	37.107	1.00	10.13	A	C
ATOM	890	OD1	ASP	A	641	39.612	58.802	37.412	1.00	8.59	A	O
ATOM	891	OD2	ASP	A	641	41.664	58.874	36.614	1.00	8.63	A	O
ATOM	892	C	ASP	A	641	39.347	62.220	35.672	1.00	11.27	A	C
ATOM	893	O	ASP	A	641	40.115	63.116	35.312	1.00	12.57	A	O
ATOM	894	N	GLN	A	642	38.423	61.681	34.874	1.00	11.26	A	N
ATOM	895	CA	GLN	A	642	38.198	62.116	33.487	1.00	9.57	A	C
ATOM	896	CB	GLN	A	642	39.048	61.292	32.500	1.00	8.69	A	C
ATOM	897	CG	GLN	A	642	40.035	62.125	31.639	1.00	5.32	A	C
ATOM	898	CD	GLN	A	642	41.163	62.752	32.447	1.00	4.15	A	C
ATOM	899	OE1	GLN	A	642	40.960	63.746	33.146	1.00	2.70	A	O
ATOM	900	NE2	GLN	A	642	42.359	62.164	32.361	1.00	2.90	A	N
ATOM	901	C	GLN	A	642	36.699	61.984	33.168	1.00	9.54	A	C
ATOM	902	O	GLN	A	642	36.280	61.562	32.082	1.00	7.27	A	O
ATOM	903	N	CYS	A	643	35.909	62.357	34.165	1.00	9.15	A	N
ATOM	904	CA	CYS	A	643	34.464	62.333	34.088	1.00	9.40	A	C
ATOM	905	CB	CYS	A	643	33.884	61.355	35.108	1.00	10.79	A	C
ATOM	906	SG	CYS	A	643	33.753	62.041	36.792	1.00	14.82	A	S
ATOM	907	C	CYS	A	643	34.038	63.735	34.471	1.00	8.44	A	C
ATOM	908	O	CYS	A	643	32.857	64.078	34.420	1.00	8.12	A	O
ATOM	909	N	LYS	A	644	35.020	64.531	34.878	1.00	7.68	A	N
ATOM	910	CA	LYS	A	644	34.783	65.900	35.288	1.00	7.75	A	C
ATOM	911	CB	LYS	A	644	35.808	66.323	36.343	1.00	9.88	A	C
ATOM	912	CG	LYS	A	644	37.264	66.008	35.972	1.00	11.67	A	C
ATOM	913	CD	LYS	A	644	38.270	66.601	36.963	1.00	12.49	A	C
ATOM	914	CE	LYS	A	644	38.090	66.006	38.350	1.00	13.22	A	C
ATOM	915	NZ	LYS	A	644	39.002	66.614	39.355	1.00	13.21	A	N
ATOM	916	C	LYS	A	644	34.844	66.832	34.088	1.00	6.70	A	C
ATOM	917	O	LYS	A	644	33.841	67.431	33.729	1.00	9.00	A	O
ATOM	918	N	HIS	A	645	36.008	66.947	33.460	1.00	4.79	A	N
ATOM	919	CA	HIS	A	645	36.161	67.823	32.304	1.00	3.28	A	C
ATOM	920	CB	HIS	A	645	37.353	67.381	31.453	1.00	3.42	A	C
ATOM	921	CG	HIS	A	645	38.614	67.169	32.230	1.00	3.61	A	C
ATOM	922	CD2	HIS	A	645	38.885	67.319	33.549	1.00	3.18	A	C
ATOM	923	ND1	HIS	A	645	39.773	66.705	31.648	1.00	3.00	A	N
ATOM	924	CE1	HIS	A	645	40.703	66.571	32.578	1.00	3.57	A	C
ATOM	925	NE2	HIS	A	645	40.189	66.936	33.739	1.00	3.50	A	N
ATOM	926	C	HIS	A	645	34.905	67.782	31.437	1.00	1.97	A	C
ATOM	927	O	HIS	A	645	34.296	68.804	31.119	1.00	2.17	A	O
ATOM	928	N	MET	A	646	34.513	66.574	31.070	1.00	0.67	A	N
ATOM	929	CA	MET	A	646	33.357	66.382	30.219	1.00	0.00	A	C
ATOM	930	CB	MET	A	646	33.197	64.892	29.935	1.00	0.00	A	C
ATOM	931	CG	MET	A	646	32.578	64.591	28.602	1.00	0.00	A	C
ATOM	932	SD	MET	A	646	32.432	62.827	28.395	1.00	0.00	A	S
ATOM	933	CE	MET	A	646	31.179	62.470	29.594	1.00	0.00	A	C
ATOM	934	C	MET	A	646	32.082	66.967	30.829	1.00	0.00	A	C

ATOM	935	O	MET	A	646	31.122	67.242	30.112	1.00	0.20	A	O
ATOM	936	N	LEU	A	647	32.080	67.146	32.150	1.00	0.00	A	N
ATOM	937	CA	LEU	A	647	30.947	67.716	32.883	1.00	0.00	A	C
ATOM	938	CB	LEU	A	647	30.724	66.954	34.182	1.00	0.00	A	C
ATOM	939	CG	LEU	A	647	29.507	67.301	35.042	1.00	0.00	A	C
ATOM	940	CD1	LEU	A	647	28.290	66.531	34.557	1.00	0.00	A	C
ATOM	941	CD2	LEU	A	647	29.782	66.927	36.485	1.00	0.00	A	C
ATOM	942	C	LEU	A	647	31.273	69.173	33.208	1.00	0.26	A	C
ATOM	943	O	LEU	A	647	30.403	69.955	33.588	1.00	0.00	A	O
ATOM	944	N	TYR	A	648	32.550	69.514	33.069	1.00	3.00	A	N
ATOM	945	CA	TYR	A	648	33.049	70.862	33.307	1.00	4.25	A	C
ATOM	946	CB	TYR	A	648	34.578	70.865	33.449	1.00	3.00	A	C
ATOM	947	CG	TYR	A	648	35.161	70.777	34.849	1.00	1.95	A	C
ATOM	948	CD1	TYR	A	648	36.522	70.993	35.052	1.00	2.30	A	C
ATOM	949	CE1	TYR	A	648	37.082	70.954	36.320	1.00	2.83	A	C
ATOM	950	CD2	TYR	A	648	34.368	70.509	35.964	1.00	2.39	A	C
ATOM	951	CE2	TYR	A	648	34.925	70.465	37.252	1.00	2.33	A	C
ATOM	952	CZ	TYR	A	648	36.283	70.693	37.411	1.00	2.60	A	C
ATOM	953	OH	TYR	A	648	36.858	70.686	38.653	1.00	2.81	A	O
ATOM	954	C	TYR	A	648	32.688	71.679	32.070	1.00	4.62	A	C
ATOM	955	O	TYR	A	648	33.209	72.782	31.868	1.00	6.78	A	O
ATOM	956	N	VAL	A	649	31.825	71.111	31.228	1.00	2.67	A	N
ATOM	957	CA	VAL	A	649	31.391	71.776	30.004	1.00	1.52	A	C
ATOM	958	CB	VAL	A	649	31.263	70.794	28.834	1.00	1.81	A	C
ATOM	959	CG1	VAL	A	649	30.428	71.395	27.735	1.00	1.28	A	C
ATOM	960	CG2	VAL	A	649	32.640	70.451	28.300	1.00	1.93	A	C
ATOM	961	C	VAL	A	649	30.043	72.380	30.252	1.00	0.68	A	C
ATOM	962	O	VAL	A	649	29.781	73.501	29.864	1.00	0.38	A	O
ATOM	963	N	SER	A	650	29.187	71.624	30.917	1.00	2.29	A	N
ATOM	964	CA	SER	A	650	27.848	72.088	31.221	1.00	3.67	A	C
ATOM	965	CB	SER	A	650	27.012	70.923	31.740	1.00	4.42	A	C
ATOM	966	OG	SER	A	650	26.741	70.022	30.686	1.00	5.99	A	O
ATOM	967	C	SER	A	650	27.783	73.259	32.197	1.00	3.84	A	C
ATOM	968	O	SER	A	650	26.908	74.098	32.089	1.00	4.82	A	O
ATOM	969	N	SER	A	651	28.692	73.323	33.156	1.00	2.84	A	N
ATOM	970	CA	SER	A	651	28.668	74.433	34.094	1.00	3.19	A	C
ATOM	971	CB	SER	A	651	29.642	74.182	35.242	1.00	4.35	A	C
ATOM	972	OG	SER	A	651	28.993	73.482	36.291	1.00	3.26	A	O
ATOM	973	C	SER	A	651	29.003	75.749	33.393	1.00	3.07	A	C
ATOM	974	O	SER	A	651	28.325	76.767	33.573	1.00	5.77	A	O
ATOM	975	N	GLU	A	652	30.049	75.729	32.585	1.00	1.49	A	N
ATOM	976	CA	GLU	A	652	30.439	76.919	31.857	1.00	0.00	A	C
ATOM	977	CB	GLU	A	652	31.703	76.621	31.041	1.00	0.00	A	C
ATOM	978	CG	GLU	A	652	32.576	77.821	30.826	1.00	0.00	A	C
ATOM	979	CD	GLU	A	652	32.591	78.723	32.041	1.00	0.00	A	C
ATOM	980	OE1	GLU	A	652	32.884	78.217	33.141	1.00	0.00	A	O
ATOM	981	OE2	GLU	A	652	32.301	79.937	31.898	1.00	0.00	A	O
ATOM	982	C	GLU	A	652	29.266	77.333	30.952	1.00	0.00	A	C
ATOM	983	O	GLU	A	652	28.910	78.498	30.864	1.00	0.06	A	O
ATOM	984	N	LEU	A	653	28.660	76.348	30.305	1.00	0.00	A	N
ATOM	985	CA	LEU	A	653	27.529	76.540	29.407	1.00	0.00	A	C
ATOM	986	CB	LEU	A	653	27.299	75.242	28.643	1.00	0.00	A	C
ATOM	987	CG	LEU	A	653	26.638	75.142	27.271	1.00	0.45	A	C
ATOM	988	CD1	LEU	A	653	25.323	75.883	27.243	1.00	0.91	A	C
ATOM	989	CD2	LEU	A	653	27.588	75.674	26.234	1.00	0.08	A	C
ATOM	990	C	LEU	A	653	26.274	76.895	30.221	1.00	0.00	A	C
ATOM	991	O	LEU	A	653	25.213	77.183	29.670	1.00	0.00	A	O
ATOM	992	N	HIS	A	654	26.401	76.869	31.541	1.00	0.13	A	N
ATOM	993	CA	HIS	A	654	25.285	77.183	32.413	1.00	0.00	A	C
ATOM	994	CB	HIS	A	654	24.956	75.982	33.290	1.00	0.00	A	C
ATOM	995	CG	HIS	A	654	23.821	76.214	34.238	1.00	0.00	A	C
ATOM	996	CD2	HIS	A	654	23.612	75.774	35.500	1.00	0.00	A	C
ATOM	997	ND1	HIS	A	654	22.713	76.960	33.902	1.00	0.00	A	N
ATOM	998	CE1	HIS	A	654	21.870	76.972	34.917	1.00	0.00	A	C
ATOM	999	NE2	HIS	A	654	22.392	76.260	35.898	1.00	0.10	A	N
ATOM	1000	C	HIS	A	654	25.681	78.362	33.265	1.00	0.00	A	C
ATOM	1001	O	HIS	A	654	24.913	78.843	34.095	1.00	0.00	A	O
ATOM	1002	N	ARG	A	655	26.914	78.804	33.069	1.00	0.00	A	N
ATOM	1003	CA	ARG	A	655	27.425	79.965	33.776	1.00	1.15	A	C
ATOM	1004	CB	ARG	A	655	28.951	79.845	33.942	1.00	3.32	A	C
ATOM	1005	CG	ARG	A	655	29.789	81.012	33.438	1.00	4.71	A	C
ATOM	1006	CD	ARG	A	655	31.144	81.015	34.111	1.00	6.49	A	C
ATOM	1007	NE	ARG	A	655	30.974	81.007	35.558	1.00	10.33	A	N
ATOM	1008	CZ	ARG	A	655	31.894	81.411	36.431	1.00	11.33	A	C
ATOM	1009	NH1	ARG	A	655	33.067	81.861	35.999	1.00	11.72	A	N
ATOM	1010	NH2	ARG	A	655	31.637	81.373	37.738	1.00	11.16	A	N
ATOM	1011	C	ARG	A	655	27.029	81.144	32.890	1.00	1.78	A	C
ATOM	1012	O	ARG	A	655	26.644	82.213	33.366	1.00	0.31	A	O
ATOM	1013	N	LEU	A	656	27.094	80.909	31.585	1.00	2.56	A	N
ATOM	1014	CA	LEU	A	656	26.723	81.909	30.606	1.00	1.97	A	C
ATOM	1015	CB	LEU	A	656	27.594	81.801	29.353	1.00	1.59	A	C

ATOM	1016	CG	LEU	A	656	29.099	81.596	29.508	1.00	0.90	A	C
ATOM	1017	CD1	LEU	A	656	29.738	81.869	28.177	1.00	1.20	A	C
ATOM	1018	CD2	LEU	A	656	29.676	82.521	30.547	1.00	1.50	A	C
ATOM	1019	C	LEU	A	656	25.281	81.667	30.213	1.00	1.35	A	C
ATOM	1020	O	LEU	A	656	24.749	82.365	29.359	1.00	1.12	A	O
ATOM	1021	N	GLN	A	657	24.652	80.669	30.825	1.00	0.96	A	N
ATOM	1022	CA	GLN	A	657	23.269	80.350	30.494	1.00	2.30	A	C
ATOM	1023	CB	GLN	A	657	22.313	81.220	31.322	1.00	4.65	A	C
ATOM	1024	CG	GLN	A	657	22.455	81.041	32.836	1.00	9.19	A	C
ATOM	1025	CD	GLN	A	657	21.835	82.186	33.650	1.00	11.69	A	C
ATOM	1026	OE1	GLN	A	657	22.004	82.263	34.878	1.00	13.17	A	O
ATOM	1027	NE2	GLN	A	657	21.118	83.077	32.967	1.00	12.66	A	N
ATOM	1028	C	GLN	A	657	23.051	80.600	28.990	1.00	1.68	A	C
ATOM	1029	O	GLN	A	657	22.030	81.155	28.583	1.00	0.00	A	O
ATOM	1030	N	VAL	A	658	24.036	80.191	28.184	1.00	1.79	A	N
ATOM	1031	CA	VAL	A	658	24.015	80.349	26.726	1.00	0.18	A	C
ATOM	1032	CB	VAL	A	658	25.066	79.453	26.021	1.00	0.00	A	C
ATOM	1033	CG1	VAL	A	658	24.974	79.652	24.515	1.00	0.00	A	C
ATOM	1034	CG2	VAL	A	658	26.465	79.775	26.518	1.00	0.00	A	C
ATOM	1035	C	VAL	A	658	22.672	79.984	26.150	1.00	0.00	A	C
ATOM	1036	O	VAL	A	658	21.945	79.191	26.722	1.00	0.00	A	O
ATOM	1037	N	SER	A	659	22.352	80.550	25.000	1.00	0.00	A	N
ATOM	1038	CA	SER	A	659	21.075	80.278	24.378	1.00	0.19	A	C
ATOM	1039	CB	SER	A	659	20.477	81.572	23.827	1.00	0.00	A	C
ATOM	1040	OG	SER	A	659	20.271	82.507	24.869	1.00	0.00	A	O
ATOM	1041	C	SER	A	659	21.213	79.255	23.275	1.00	2.56	A	C
ATOM	1042	O	SER	A	659	22.321	79.008	22.785	1.00	2.52	A	O
ATOM	1043	N	TYR	A	660	20.075	78.666	22.895	1.00	4.88	A	N
ATOM	1044	CA	TYR	A	660	20.004	77.644	21.841	1.00	5.35	A	C
ATOM	1045	CB	TYR	A	660	18.602	77.032	21.800	1.00	4.05	A	C
ATOM	1046	CG	TYR	A	660	18.432	75.932	20.786	1.00	0.56	A	C
ATOM	1047	CD1	TYR	A	660	19.028	74.696	20.964	1.00	0.60	A	C
ATOM	1048	CE1	TYR	A	660	18.903	73.703	20.027	1.00	1.19	A	C
ATOM	1049	CD2	TYR	A	660	17.697	76.142	19.634	1.00	0.85	A	C
ATOM	1050	CE2	TYR	A	660	17.567	75.151	18.692	1.00	2.08	A	C
ATOM	1051	CZ	TYR	A	660	18.176	73.938	18.895	1.00	1.32	A	C
ATOM	1052	OH	TYR	A	660	18.079	72.971	17.934	1.00	2.12	A	O
ATOM	1053	C	TYR	A	660	20.360	78.194	20.466	1.00	5.76	A	C
ATOM	1054	O	TYR	A	660	21.144	77.601	19.737	1.00	6.61	A	O
ATOM	1055	N	GLU	A	661	19.777	79.324	20.103	1.00	5.56	A	N
ATOM	1056	CA	GLU	A	661	20.100	79.908	18.821	1.00	6.01	A	C
ATOM	1057	CB	GLU	A	661	19.180	81.103	18.532	1.00	6.90	A	C
ATOM	1058	CG	GLU	A	661	17.671	80.830	18.831	1.00	7.00	A	C
ATOM	1059	CD	GLU	A	661	17.043	79.632	18.070	1.00	5.83	A	C
ATOM	1060	OE1	GLU	A	661	15.900	79.257	18.405	1.00	5.11	A	O
ATOM	1061	OE2	GLU	A	661	17.660	79.068	17.141	1.00	5.63	A	O
ATOM	1062	C	GLU	A	661	21.582	80.311	18.866	1.00	6.34	A	C
ATOM	1063	O	GLU	A	661	22.209	80.494	17.824	1.00	7.80	A	O
ATOM	1064	N	GLU	A	662	22.138	80.419	20.077	1.00	5.60	A	N
ATOM	1065	CA	GLU	A	662	23.560	80.754	20.277	1.00	4.68	A	C
ATOM	1066	CB	GLU	A	662	23.824	81.254	21.701	1.00	3.42	A	C
ATOM	1067	CG	GLU	A	662	23.486	82.709	21.962	1.00	3.57	A	C
ATOM	1068	CD	GLU	A	662	23.857	83.144	23.370	1.00	3.89	A	C
ATOM	1069	OE1	GLU	A	662	23.214	82.683	24.330	1.00	3.46	A	O
ATOM	1070	OE2	GLU	A	662	24.801	83.942	23.516	1.00	3.60	A	O
ATOM	1071	C	GLU	A	662	24.433	79.522	20.064	1.00	3.86	A	C
ATOM	1072	O	GLU	A	662	25.533	79.611	19.525	1.00	2.57	A	O
ATOM	1073	N	TYR	A	663	23.911	78.381	20.516	1.00	2.92	A	N
ATOM	1074	CA	TYR	A	663	24.547	77.058	20.455	1.00	1.36	A	C
ATOM	1075	CB	TYR	A	663	23.699	76.091	21.294	1.00	1.01	A	C
ATOM	1076	CG	TYR	A	663	23.939	74.609	21.084	1.00	0.78	A	C
ATOM	1077	CD1	TYR	A	663	25.119	74.009	21.500	1.00	0.95	A	C
ATOM	1078	CE1	TYR	A	663	25.319	72.641	21.351	1.00	1.16	A	C
ATOM	1079	CD2	TYR	A	663	22.963	73.801	20.508	1.00	0.00	A	C
ATOM	1080	CE2	TYR	A	663	23.151	72.442	20.354	1.00	0.07	A	C
ATOM	1081	CZ	TYR	A	663	24.330	71.864	20.777	1.00	1.11	A	C
ATOM	1082	OH	TYR	A	663	24.523	70.507	20.633	1.00	2.23	A	O
ATOM	1083	C	TYR	A	663	24.744	76.499	19.046	1.00	0.18	A	C
ATOM	1084	O	TYR	A	663	25.817	76.057	18.686	1.00	1.22	A	O
ATOM	1085	N	LEU	A	664	23.692	76.518	18.252	1.00	0.00	A	N
ATOM	1086	CA	LEU	A	664	23.769	75.996	16.907	1.00	0.00	A	C
ATOM	1087	CB	LEU	A	664	22.412	76.141	16.194	1.00	0.00	A	C
ATOM	1088	CG	LEU	A	664	21.059	75.657	16.755	1.00	0.00	A	C
ATOM	1089	CD1	LEU	A	664	20.091	75.609	15.595	1.00	0.00	A	C
ATOM	1090	CD2	LEU	A	664	21.139	74.285	17.400	1.00	0.00	A	C
ATOM	1091	C	LEU	A	664	24.839	76.711	16.110	1.00	0.00	A	C
ATOM	1092	O	LEU	A	664	25.418	76.143	15.206	1.00	1.46	A	O
ATOM	1093	N	CYS	A	665	25.093	77.970	16.433	1.00	0.00	A	N
ATOM	1094	CA	CYS	A	665	26.113	78.742	15.727	1.00	0.60	A	C
ATOM	1095	CB	CYS	A	665	25.833	80.235	15.826	1.00	2.53	A	C
ATOM	1096	SG	CYS	A	665	25.517	80.981	14.234	1.00	6.81	A	S

ATOM	1097	C	CYS	A	665	27.441	78.456	16.369	1.00	0.80	A	C
ATOM	1098	O	CYS	A	665	28.445	78.258	15.696	1.00	1.03	A	O
ATOM	1099	N	MET	A	666	27.418	78.434	17.694	1.00	2.06	A	N
ATOM	1100	CA	MET	A	666	28.593	78.165	18.500	1.00	2.69	A	C
ATOM	1101	CB	MET	A	666	28.192	78.099	19.964	1.00	1.39	A	C
ATOM	1102	CG	MET	A	666	29.192	78.701	20.895	1.00	1.51	A	C
ATOM	1103	SD	MET	A	666	28.361	79.316	22.353	1.00	0.80	A	S
ATOM	1104	CE	MET	A	666	28.430	77.902	23.452	1.00	0.75	A	C
ATOM	1105	C	MET	A	666	29.238	76.853	18.084	1.00	2.96	A	C
ATOM	1106	O	MET	A	666	30.419	76.815	17.754	1.00	3.84	A	O
ATOM	1107	N	LYS	A	667	28.461	75.777	18.085	1.00	2.06	A	N
ATOM	1108	CA	LYS	A	667	28.991	74.475	17.705	1.00	1.40	A	C
ATOM	1109	CB	LYS	A	667	27.959	73.371	17.964	1.00	3.10	A	C
ATOM	1110	CG	LYS	A	667	28.540	71.960	18.024	1.00	2.32	A	C
ATOM	1111	CD	LYS	A	667	27.508	70.938	17.606	1.00	1.75	A	C
ATOM	1112	CE	LYS	A	667	27.127	71.129	16.136	1.00	2.03	A	C
ATOM	1113	NZ	LYS	A	667	26.050	70.202	15.668	1.00	3.00	A	N
ATOM	1114	C	LYS	A	667	29.431	74.446	16.243	1.00	0.99	A	C
ATOM	1115	O	LYS	A	667	30.437	73.819	15.930	1.00	3.23	A	O
ATOM	1116	N	THR	A	668	28.711	75.112	15.343	1.00	0.00	A	N
ATOM	1117	CA	THR	A	668	29.141	75.093	13.945	1.00	0.00	A	C
ATOM	1118	CB	THR	A	668	28.281	75.972	13.027	1.00	0.00	A	C
ATOM	1119	OG1	THR	A	668	26.935	75.504	13.018	1.00	0.00	A	O
ATOM	1120	CG2	THR	A	668	28.811	75.908	11.604	1.00	0.00	A	C
ATOM	1121	C	THR	A	668	30.575	75.593	13.802	1.00	0.00	A	C
ATOM	1122	O	THR	A	668	31.337	75.092	12.975	1.00	0.00	A	O
ATOM	1123	N	LEU	A	669	30.931	76.593	14.603	1.00	0.00	A	N
ATOM	1124	CA	LEU	A	669	32.268	77.166	14.559	1.00	0.00	A	C
ATOM	1125	CB	LEU	A	669	32.268	78.597	15.098	1.00	0.00	A	C
ATOM	1126	CG	LEU	A	669	31.718	79.668	14.143	1.00	0.69	A	C
ATOM	1127	CD1	LEU	A	669	31.802	81.036	14.796	1.00	1.66	A	C
ATOM	1128	CD2	LEU	A	669	32.504	79.663	12.839	1.00	0.53	A	C
ATOM	1129	C	LEU	A	669	33.240	76.322	15.342	1.00	0.00	A	C
ATOM	1130	O	LEU	A	669	34.433	76.607	15.385	1.00	0.00	A	O
ATOM	1131	N	LEU	A	670	32.731	75.274	15.968	1.00	0.43	A	N
ATOM	1132	CA	LEU	A	670	33.601	74.395	16.713	1.00	1.04	A	C
ATOM	1133	CB	LEU	A	670	32.816	73.594	17.737	1.00	0.78	A	C
ATOM	1134	CG	LEU	A	670	33.617	73.572	19.031	1.00	2.00	A	C
ATOM	1135	CD1	LEU	A	670	32.855	72.877	20.131	1.00	1.96	A	C
ATOM	1136	CD2	LEU	A	670	34.928	72.892	18.770	1.00	2.92	A	C
ATOM	1137	C	LEU	A	670	34.214	73.471	15.685	1.00	1.90	A	C
ATOM	1138	O	LEU	A	670	35.303	72.938	15.880	1.00	3.58	A	O
ATOM	1139	N	LEU	A	671	33.497	73.298	14.579	1.00	2.26	A	N
ATOM	1140	CA	LEU	A	671	33.948	72.454	13.487	1.00	3.12	A	C
ATOM	1141	CB	LEU	A	671	32.834	72.258	12.461	1.00	3.12	A	C
ATOM	1142	CG	LEU	A	671	33.233	71.504	11.193	1.00	2.58	A	C
ATOM	1143	CD1	LEU	A	671	32.002	70.911	10.539	1.00	2.66	A	C
ATOM	1144	CD2	LEU	A	671	33.952	72.437	10.245	1.00	1.15	A	C
ATOM	1145	C	LEU	A	671	35.114	73.143	12.832	1.00	3.75	A	C
ATOM	1146	O	LEU	A	671	36.238	72.641	12.854	1.00	5.20	A	O
ATOM	1147	N	LEU	A	672	34.832	74.307	12.257	1.00	4.27	A	N
ATOM	1148	CA	LEU	A	672	35.837	75.122	11.570	1.00	3.16	A	C
ATOM	1149	CB	LEU	A	672	35.212	76.438	11.096	1.00	3.24	A	C
ATOM	1150	CG	LEU	A	672	34.063	76.359	10.093	1.00	2.96	A	C
ATOM	1151	CD1	LEU	A	672	33.512	77.750	9.881	1.00	2.32	A	C
ATOM	1152	CD2	LEU	A	672	34.545	75.750	8.781	1.00	3.56	A	C
ATOM	1153	C	LEU	A	672	37.065	75.451	12.411	1.00	2.37	A	C
ATOM	1154	O	LEU	A	672	38.167	75.529	11.895	1.00	1.83	A	O
ATOM	1155	N	SER	A	673	36.872	75.634	13.708	1.00	0.69	A	N
ATOM	1156	CA	SER	A	673	37.978	75.988	14.580	1.00	0.34	A	C
ATOM	1157	CB	SER	A	673	37.437	76.488	15.931	1.00	2.28	A	C
ATOM	1158	OG	SER	A	673	36.744	77.724	15.801	1.00	3.07	A	O
ATOM	1159	C	SER	A	673	39.078	74.946	14.812	1.00	0.28	A	C
ATOM	1160	O	SER	A	673	39.189	74.370	15.891	1.00	0.00	A	O
ATOM	1161	N	SER	A	674	39.890	74.734	13.780	1.00	0.46	A	N
ATOM	1162	CA	SER	A	674	41.054	73.833	13.790	1.00	0.28	A	C
ATOM	1163	CB	SER	A	674	40.795	72.540	14.569	1.00	0.00	A	C
ATOM	1164	OG	SER	A	674	42.004	72.020	15.097	1.00	0.00	A	O
ATOM	1165	C	SER	A	674	41.386	73.511	12.343	1.00	0.00	A	C
ATOM	1166	O	SER	A	674	40.692	72.720	11.703	1.00	0.00	A	C
ATOM	1167	N	VAL	A	675	42.431	74.158	11.832	1.00	0.00	A	O
ATOM	1168	CA	VAL	A	675	42.878	73.984	10.457	1.00	0.93	A	N
ATOM	1169	CB	VAL	A	675	42.832	75.323	9.732	1.00	5.42	A	C
ATOM	1170	CG1	VAL	A	675	44.233	75.875	9.559	1.00	6.28	A	C
ATOM	1171	CG2	VAL	A	675	42.107	75.173	8.409	1.00	6.64	A	C
ATOM	1172	C	VAL	A	675	44.306	73.459	10.493	1.00	0.00	A	C
ATOM	1173	O	VAL	A	675	44.927	73.455	11.541	1.00	4.03	A	O
ATOM	1174	N	PRO	A	676	44.855	73.017	9.359	1.00	0.00	A	N
ATOM	1175	CD	PRO	A	676	44.300	72.829	8.019	1.00	0.00	A	C
ATOM	1176	CA	PRO	A	676	46.227	72.512	9.418	1.00	0.00	A	C
ATOM	1177	CB	PRO	A	676	46.368	71.715	8.128	1.00	0.00	A	C

ATOM	1178	CG	PRO	A	676	44.966	71.562	7.620	1.00	0.00	A	C
ATOM	1179	C	PRO	A	676	47.195	73.679	9.454	1.00	0.02	A	C
ATOM	1180	O	PRO	A	676	47.003	74.664	8.738	1.00	0.92	A	O
ATOM	1181	N	LYS	A	677	48.238	73.578	10.273	1.00	2.19	A	N
ATOM	1182	CA	LYS	A	677	49.216	74.651	10.371	1.00	3.58	A	C
ATOM	1183	CB	LYS	A	677	50.455	74.179	11.132	1.00	3.72	A	C
ATOM	1184	CG	LYS	A	677	51.264	75.311	11.779	1.00	4.97	A	C
ATOM	1185	CD	LYS	A	677	52.254	74.788	12.815	1.00	4.83	A	C
ATOM	1186	CE	LYS	A	677	53.452	74.162	12.165	1.00	4.63	A	C
ATOM	1187	NZ	LYS	A	677	53.067	73.161	11.157	1.00	5.52	A	N
ATOM	1188	C	LYS	A	677	49.600	75.090	8.971	1.00	4.37	A	C
ATOM	1189	O	LYS	A	677	50.149	76.159	8.781	1.00	4.76	A	O
ATOM	1190	N	ASP	A	678	49.315	74.248	7.990	1.00	5.33	A	N
ATOM	1191	CA	ASP	A	678	49.609	74.579	6.611	1.00	7.61	A	C
ATOM	1192	CB	ASP	A	678	49.756	73.321	5.777	1.00	8.33	A	C
ATOM	1193	CG	ASP	A	678	50.993	72.563	6.114	1.00	10.02	A	C
ATOM	1194	OD1	ASP	A	678	52.091	73.092	5.814	1.00	9.04	A	O
ATOM	1195	OD2	ASP	A	678	50.867	71.455	6.688	1.00	9.62	A	O
ATOM	1196	C	ASP	A	678	48.461	75.388	6.060	1.00	8.53	A	C
ATOM	1197	O	ASP	A	678	48.614	76.570	5.739	1.00	10.53	A	O
ATOM	1198	N	GLY	A	679	47.306	74.740	5.955	1.00	8.84	A	N
ATOM	1199	CA	GLY	A	679	46.128	75.393	5.424	1.00	7.61	A	C
ATOM	1200	C	GLY	A	679	45.562	74.540	4.314	1.00	6.93	A	C
ATOM	1201	O	GLY	A	679	46.294	74.093	3.440	1.00	7.75	A	O
ATOM	1202	N	LEU	A	680	44.254	74.318	4.357	1.00	6.20	A	N
ATOM	1203	CA	LEU	A	680	43.544	73.500	3.374	1.00	6.37	A	C
ATOM	1204	CB	LEU	A	680	42.031	73.597	3.614	1.00	5.74	A	C
ATOM	1205	CG	LEU	A	680	41.465	73.871	5.011	1.00	5.30	A	C
ATOM	1206	CD1	LEU	A	680	39.991	74.217	4.872	1.00	4.49	A	C
ATOM	1207	CD2	LEU	A	680	41.669	72.676	5.926	1.00	4.78	A	C
ATOM	1208	C	LEU	A	680	43.824	73.922	1.930	1.00	6.34	A	C
ATOM	1209	O	LEU	A	680	44.512	74.913	1.681	1.00	7.33	A	O
ATOM	1210	N	LYS	A	681	43.284	73.160	0.983	1.00	5.96	A	N
ATOM	1211	CA	LYS	A	681	43.435	73.483	-0.426	1.00	4.50	A	C
ATOM	1212	CB	LYS	A	681	43.153	72.264	-1.299	1.00	2.91	A	C
ATOM	1213	CG	LYS	A	681	44.159	71.139	-1.191	1.00	3.18	A	C
ATOM	1214	CD	LYS	A	681	43.884	70.058	-2.248	1.00	1.53	A	C
ATOM	1215	CE	LYS	A	681	44.769	68.849	-2.043	1.00	0.52	A	C
ATOM	1216	NZ	LYS	A	681	44.576	68.291	-0.680	1.00	0.00	A	N
ATOM	1217	C	LYS	A	681	42.403	74.552	-0.761	1.00	3.86	A	C
ATOM	1218	O	LYS	A	681	42.267	74.964	-1.909	1.00	5.00	A	O
ATOM	1219	N	SER	A	682	41.670	75.010	0.242	1.00	2.21	A	N
ATOM	1220	CA	SER	A	682	40.637	75.987	-0.020	1.00	1.48	A	C
ATOM	1221	CB	SER	A	682	39.263	75.317	0.057	1.00	0.59	A	C
ATOM	1222	OG	SER	A	682	39.087	74.339	-0.955	1.00	0.00	A	O
ATOM	1223	C	SER	A	682	40.651	77.183	0.898	1.00	1.32	A	C
ATOM	1224	O	SER	A	682	39.840	78.083	0.727	1.00	2.02	A	O
ATOM	1225	N	GLN	A	683	41.558	77.200	1.867	1.00	0.99	A	N
ATOM	1226	CA	GLN	A	683	41.645	78.305	2.818	1.00	0.53	A	C
ATOM	1227	CB	GLN	A	683	43.113	78.689	3.037	1.00	0.00	A	C
ATOM	1228	CG	GLN	A	683	43.392	79.291	4.402	1.00	0.00	A	C
ATOM	1229	CD	GLN	A	683	43.071	78.337	5.540	1.00	0.00	A	C
ATOM	1230	OE1	GLN	A	683	43.144	78.695	6.722	1.00	0.00	A	O
ATOM	1231	NE2	GLN	A	683	42.718	77.112	5.189	1.00	0.00	A	N
ATOM	1232	C	GLN	A	683	40.825	79.526	2.362	1.00	1.24	A	C
ATOM	1233	O	GLN	A	683	39.857	79.901	3.018	1.00	0.00	A	O
ATOM	1234	N	GLU	A	684	41.200	80.118	1.228	1.00	2.28	A	N
ATOM	1235	CA	GLU	A	684	40.503	81.286	0.669	1.00	3.12	A	C
ATOM	1236	CB	GLU	A	684	40.747	81.391	-0.843	1.00	2.28	A	C
ATOM	1237	CG	GLU	A	684	42.197	81.390	-1.222	1.00	4.18	A	C
ATOM	1238	CD	GLU	A	684	42.434	80.826	-2.600	1.00	5.76	A	C
ATOM	1239	OE1	GLU	A	684	41.763	79.840	-2.974	1.00	6.78	A	O
ATOM	1240	OE2	GLU	A	684	43.312	81.356	-3.307	1.00	7.49	A	O
ATOM	1241	C	GLU	A	684	39.015	81.140	0.920	1.00	4.14	A	C
ATOM	1242	O	GLU	A	684	38.393	81.969	1.578	1.00	2.58	A	O
ATOM	1243	N	LEU	A	685	38.452	80.073	0.376	1.00	6.60	A	N
ATOM	1244	CA	LEU	A	685	37.044	79.791	0.551	1.00	9.37	A	C
ATOM	1245	CB	LEU	A	685	36.668	78.494	-0.188	1.00	13.24	A	C
ATOM	1246	CG	LEU	A	685	36.827	78.467	-1.727	1.00	16.37	A	C
ATOM	1247	CD1	LEU	A	685	38.302	78.646	-2.122	1.00	17.41	A	C
ATOM	1248	CD2	LEU	A	685	36.283	77.144	-2.293	1.00	17.81	A	C
ATOM	1249	C	LEU	A	685	36.787	79.664	2.057	1.00	8.74	A	C
ATOM	1250	O	LEU	A	685	36.076	80.493	2.636	1.00	10.87	A	O
ATOM	1251	N	PHE	A	686	37.382	78.656	2.692	1.00	7.27	A	N
ATOM	1252	CA	PHE	A	686	37.205	78.441	4.128	1.00	6.78	A	C
ATOM	1253	CB	PHE	A	686	38.358	77.605	4.673	1.00	8.71	A	C
ATOM	1254	CG	PHE	A	686	38.498	77.668	6.168	1.00	9.98	A	C
ATOM	1255	CD1	PHE	A	686	37.497	77.171	6.995	1.00	8.89	A	C
ATOM	1256	CD2	PHE	A	686	39.622	78.253	6.748	1.00	9.64	A	C
ATOM	1257	CE1	PHE	A	686	37.612	77.253	8.380	1.00	9.75	A	C
ATOM	1258	CE2	PHE	A	686	39.748	78.342	8.128	1.00	9.87	A	C

ATOM	1259	CZ	PHE	A	686	38.741	77.843	8.948	1.00	10.36	A	C
ATOM	1260	C	PHE	A	686	37.072	79.715	4.973	1.00	5.41	A	C
ATOM	1261	O	PHE	A	686	36.207	79.797	5.847	1.00	4.79	A	C
ATOM	1262	N	ASP	A	687	37.943	80.691	4.715	1.00	4.49	A	N
ATOM	1263	CA	ASP	A	687	37.952	81.967	5.442	1.00	3.91	A	C
ATOM	1264	CB	ASP	A	687	38.916	82.970	4.780	1.00	6.22	A	C
ATOM	1265	CG	ASP	A	687	40.382	82.530	4.828	1.00	8.37	A	C
ATOM	1266	OD1	ASP	A	687	40.886	82.221	5.930	1.00	9.89	A	O
ATOM	1267	OD2	ASP	A	687	41.037	82.515	3.759	1.00	9.81	A	O
ATOM	1268	C	ASP	A	687	36.566	82.593	5.458	1.00	3.02	A	C
ATOM	1269	O	ASP	A	687	36.060	83.014	6.496	1.00	0.75	A	O
ATOM	1270	N	GLU	A	688	35.973	82.663	4.274	1.00	3.44	A	N
ATOM	1271	CA	GLU	A	688	34.652	83.235	4.094	1.00	3.78	A	C
ATOM	1272	CB	GLU	A	688	34.243	83.139	2.625	1.00	5.05	A	C
ATOM	1273	CG	GLU	A	688	35.381	83.451	1.666	1.00	9.77	A	C
ATOM	1274	CD	GLU	A	688	35.082	83.097	0.210	1.00	12.90	A	C
ATOM	1275	OE1	GLU	A	688	36.017	83.188	-0.629	1.00	14.16	A	O
ATOM	1276	OE2	GLU	A	688	33.920	82.734	-0.097	1.00	14.54	A	O
ATOM	1277	C	GLU	A	688	33.681	82.442	4.942	1.00	3.21	A	C
ATOM	1278	O	GLU	A	688	33.117	82.963	5.901	1.00	2.90	A	O
ATOM	1279	N	ILE	A	689	33.529	81.166	4.588	1.00	2.78	A	N
ATOM	1280	CA	ILE	A	689	32.609	80.236	5.245	1.00	3.97	A	C
ATOM	1281	CB	ILE	A	689	32.710	78.827	4.569	1.00	5.94	A	C
ATOM	1282	CG2	ILE	A	689	34.063	78.223	4.835	1.00	6.25	A	C
ATOM	1283	CG1	ILE	A	689	31.596	77.901	5.072	1.00	4.28	A	C
ATOM	1284	CD1	ILE	A	689	31.420	76.652	4.226	1.00	2.06	A	C
ATOM	1285	C	ILE	A	689	32.720	80.113	6.774	1.00	4.08	A	C
ATOM	1286	O	ILE	A	689	32.010	79.322	7.396	1.00	4.53	A	O
ATOM	1287	N	ARG	A	690	33.591	80.908	7.380	1.00	4.27	A	N
ATOM	1288	CA	ARG	A	690	33.752	80.888	8.827	1.00	5.29	A	C
ATOM	1289	CB	ARG	A	690	35.207	80.566	9.198	1.00	5.81	A	C
ATOM	1290	CG	ARG	A	690	35.521	80.652	10.692	1.00	4.04	A	C
ATOM	1291	CD	ARG	A	690	36.888	80.066	11.028	1.00	2.22	A	C
ATOM	1292	NE	ARG	A	690	37.550	80.839	12.072	1.00	0.00	A	N
ATOM	1293	CZ	ARG	A	690	38.368	81.858	11.836	1.00	0.00	A	N
ATOM	1294	NH1	ARG	A	690	38.636	82.222	10.588	1.00	0.00	A	N
ATOM	1295	NH2	ARG	A	690	38.902	82.525	12.848	1.00	0.00	A	N
ATOM	1296	C	ARG	A	690	33.338	82.249	9.383	1.00	6.52	A	C
ATOM	1297	O	ARG	A	690	32.415	82.340	10.199	1.00	7.32	A	O
ATOM	1298	N	MET	A	691	34.018	83.304	8.937	1.00	7.37	A	N
ATOM	1299	CA	MET	A	691	33.698	84.658	9.369	1.00	7.80	A	C
ATOM	1300	CB	MET	A	691	34.406	85.682	8.486	1.00	9.85	A	C
ATOM	1301	CG	MET	A	691	35.903	85.769	8.634	1.00	14.12	A	C
ATOM	1302	SD	MET	A	691	36.574	86.503	7.120	1.00	17.44	A	S
ATOM	1303	CE	MET	A	691	38.346	86.035	7.212	1.00	16.54	A	C
ATOM	1304	C	MET	A	691	32.194	84.843	9.218	1.00	6.50	A	C
ATOM	1305	O	MET	A	691	31.588	85.656	9.910	1.00	5.11	A	O
ATOM	1306	N	THR	A	692	31.605	84.086	8.294	1.00	5.25	A	N
ATOM	1307	CA	THR	A	692	30.171	84.142	8.039	1.00	5.05	A	C
ATOM	1308	CB	THR	A	692	29.758	83.292	6.844	1.00	6.07	A	C
ATOM	1309	OG1	THR	A	692	28.330	83.216	6.785	1.00	5.94	A	O
ATOM	1310	CG2	THR	A	692	30.291	81.898	6.991	1.00	7.23	A	C
ATOM	1311	C	THR	A	692	29.363	83.639	9.211	1.00	4.25	A	C
ATOM	1312	O	THR	A	692	28.444	84.307	9.665	1.00	5.98	A	O
ATOM	1313	N	TYR	A	693	29.687	82.459	9.705	1.00	2.96	A	N
ATOM	1314	CA	TYR	A	693	28.928	81.931	10.819	1.00	2.04	A	C
ATOM	1315	CB	TYR	A	693	29.353	80.479	11.116	1.00	1.85	A	C
ATOM	1316	CG	TYR	A	693	28.580	79.558	10.224	1.00	0.00	A	C
ATOM	1317	CD1	TYR	A	693	27.231	79.323	10.466	1.00	0.00	A	C
ATOM	1318	CE1	TYR	A	693	26.443	78.672	9.550	1.00	0.00	A	C
ATOM	1319	CD2	TYR	A	693	29.127	79.096	9.036	1.00	0.00	A	C
ATOM	1320	CE2	TYR	A	693	28.347	78.447	8.106	1.00	0.00	A	C
ATOM	1321	CZ	TYR	A	693	27.001	78.241	8.367	1.00	0.00	A	C
ATOM	1322	OH	TYR	A	693	26.201	77.634	7.433	1.00	0.00	A	O
ATOM	1323	C	TYR	A	693	29.050	82.834	12.019	1.00	2.77	A	C
ATOM	1324	O	TYR	A	693	28.086	83.035	12.757	1.00	0.02	A	O
ATOM	1325	N	ILE	A	694	30.233	83.406	12.182	1.00	4.12	A	N
ATOM	1326	CA	ILE	A	694	30.481	84.311	13.289	1.00	5.42	A	C
ATOM	1327	CB	ILE	A	694	31.855	84.948	13.171	1.00	5.41	A	C
ATOM	1328	CG2	ILE	A	694	32.170	85.729	14.439	1.00	5.30	A	C
ATOM	1329	CG1	ILE	A	694	32.886	83.848	12.934	1.00	6.28	A	C
ATOM	1330	CD1	ILE	A	694	34.232	84.349	12.535	1.00	8.00	A	C
ATOM	1331	C	ILE	A	694	29.411	85.392	13.308	1.00	6.36	A	C
ATOM	1332	O	ILE	A	694	28.818	85.651	14.353	1.00	7.31	A	O
ATOM	1333	N	LYS	A	695	29.152	86.019	12.164	1.00	6.63	A	N
ATOM	1334	CA	LYS	A	695	28.110	87.038	12.123	1.00	6.60	A	C
ATOM	1335	CB	LYS	A	695	27.915	87.602	10.704	1.00	6.97	A	C
ATOM	1336	CG	LYS	A	695	28.139	89.124	10.604	1.00	4.44	A	C
ATOM	1337	CD	LYS	A	695	27.684	89.708	9.264	1.00	3.90	A	C
ATOM	1338	CE	LYS	A	695	28.315	89.018	8.059	1.00	3.42	A	C
ATOM	1339	NZ	LYS	A	695	29.808	89.062	8.047	1.00	3.30	A	N

ATOM	1340	C	LYS	A	695	26.821	86.365	12.594	1.00	6.48	A	C
ATOM	1341	O	LYS	A	695	26.084	86.915	13.413	1.00	7.04	A	O
ATOM	1342	N	GLU	A	696	26.561	85.163	12.090	1.00	5.15	A	N
ATOM	1343	CA	GLU	A	696	25.358	84.453	12.480	1.00	4.91	A	C
ATOM	1344	CB	GLU	A	696	25.308	83.072	11.846	1.00	6.18	A	C
ATOM	1345	CG	GLU	A	696	23.923	82.711	11.379	1.00	5.89	A	C
ATOM	1346	CD	GLU	A	696	23.389	83.742	10.414	1.00	7.15	A	C
ATOM	1347	OE1	GLU	A	696	24.016	83.932	9.355	1.00	7.26	A	O
ATOM	1348	OE2	GLU	A	696	22.352	84.371	10.715	1.00	7.38	A	O
ATOM	1349	C	GLU	A	696	25.355	84.327	13.985	1.00	4.78	A	C
ATOM	1350	O	GLU	A	696	24.300	84.354	14.619	1.00	3.74	A	O
ATOM	1351	N	LEU	A	697	26.542	84.172	14.558	1.00	4.90	A	N
ATOM	1352	CA	LEU	A	697	26.665	84.076	16.004	1.00	3.42	A	C
ATOM	1353	CB	LEU	A	697	28.061	83.583	16.393	1.00	2.36	A	C
ATOM	1354	CG	LEU	A	697	28.488	83.730	17.856	1.00	2.13	A	C
ATOM	1355	CD1	LEU	A	697	27.527	82.994	18.743	1.00	1.88	A	C
ATOM	1356	CD2	LEU	A	697	29.894	83.198	18.043	1.00	2.22	A	C
ATOM	1357	C	LEU	A	697	26.461	85.498	16.483	1.00	2.99	A	C
ATOM	1358	O	LEU	A	697	25.926	85.745	17.559	1.00	2.83	A	O
ATOM	1359	N	GLY	A	698	26.879	86.435	15.646	1.00	1.86	A	N
ATOM	1360	CA	GLY	A	698	26.754	87.837	15.978	1.00	4.30	A	C
ATOM	1361	C	GLY	A	698	25.322	88.326	15.977	1.00	4.91	A	C
ATOM	1362	O	GLY	A	698	25.051	89.503	16.220	1.00	4.83	A	O
ATOM	1363	N	LYS	A	699	24.395	87.431	15.688	1.00	4.49	A	N
ATOM	1364	CA	LYS	A	699	23.001	87.814	15.684	1.00	4.89	A	C
ATOM	1365	CB	LYS	A	699	22.405	87.520	14.312	1.00	4.61	A	C
ATOM	1366	CG	LYS	A	699	23.112	88.273	13.202	1.00	2.40	A	C
ATOM	1367	CD	LYS	A	699	22.473	88.024	11.848	1.00	0.60	A	C
ATOM	1368	CE	LYS	A	699	23.158	88.853	10.768	1.00	0.00	A	C
ATOM	1369	NZ	LYS	A	699	23.133	90.329	11.058	1.00	0.00	A	N
ATOM	1370	C	LYS	A	699	22.313	87.020	16.788	1.00	5.36	A	C
ATOM	1371	O	LYS	A	699	21.224	87.363	17.247	1.00	6.37	A	O
ATOM	1372	N	ALA	A	700	23.005	85.975	17.228	1.00	5.81	A	N
ATOM	1373	CA	ALA	A	700	22.545	85.072	18.270	1.00	4.96	A	C
ATOM	1374	CB	ALA	A	700	23.464	83.866	18.318	1.00	5.62	A	C
ATOM	1375	C	ALA	A	700	22.488	85.730	19.643	1.00	3.72	A	C
ATOM	1376	O	ALA	A	700	21.599	85.431	20.445	1.00	3.83	A	O
ATOM	1377	N	ILE	A	701	23.457	86.607	19.909	1.00	1.51	A	N
ATOM	1378	CA	ILE	A	701	23.557	87.322	21.181	1.00	0.37	A	C
ATOM	1379	CB	ILE	A	701	24.972	87.845	21.440	1.00	0.12	A	C
ATOM	1380	CG2	ILE	A	701	24.987	88.636	22.732	1.00	0.00	A	C
ATOM	1381	CG1	ILE	A	701	25.973	86.690	21.477	1.00	0.00	A	C
ATOM	1382	CD1	ILE	A	701	27.405	87.137	21.625	1.00	0.00	A	C
ATOM	1383	C	ILE	A	701	22.676	88.531	21.089	1.00	0.03	A	C
ATOM	1384	O	ILE	A	701	22.409	89.200	22.076	1.00	0.04	A	O
ATOM	1385	N	VAL	A	702	22.237	88.807	19.874	1.00	0.28	A	N
ATOM	1386	CA	VAL	A	702	21.392	89.949	19.604	1.00	0.00	A	C
ATOM	1387	CB	VAL	A	702	21.724	90.526	18.198	1.00	0.00	A	C
ATOM	1388	CG1	VAL	A	702	20.465	90.915	17.451	1.00	0.00	A	C
ATOM	1389	CG2	VAL	A	702	22.644	91.723	18.356	1.00	0.00	A	C
ATOM	1390	C	VAL	A	702	19.916	89.585	19.728	1.00	0.00	A	C
ATOM	1391	O	VAL	A	702	19.146	90.333	20.333	1.00	0.00	A	O
ATOM	1392	N	LYS	A	703	19.534	88.433	19.173	1.00	0.00	A	N
ATOM	1393	CA	LYS	A	703	18.149	87.970	19.216	1.00	0.61	A	C
ATOM	1394	CB	LYS	A	703	18.063	86.511	18.779	1.00	0.00	A	C
ATOM	1395	CG	LYS	A	703	18.473	86.255	17.341	1.00	0.00	A	C
ATOM	1396	CD	LYS	A	703	17.368	86.597	16.366	1.00	0.00	A	C
ATOM	1397	CE	LYS	A	703	16.189	85.653	16.500	1.00	0.00	A	C
ATOM	1398	NZ	LYS	A	703	15.097	85.982	15.536	1.00	0.00	A	N
ATOM	1399	C	LYS	A	703	17.605	88.115	20.625	1.00	1.66	A	C
ATOM	1400	O	LYS	A	703	16.544	88.693	20.845	1.00	1.83	A	O
ATOM	1401	N	ARG	A	704	18.341	87.589	21.588	1.00	2.59	A	N
ATOM	1402	CA	ARG	A	704	17.935	87.680	22.976	1.00	3.86	A	C
ATOM	1403	CB	ARG	A	704	18.716	86.631	23.761	1.00	1.08	A	C
ATOM	1404	CG	ARG	A	704	18.570	85.238	23.136	1.00	0.00	A	C
ATOM	1405	CD	ARG	A	704	17.175	84.623	23.428	1.00	0.29	A	C
ATOM	1406	NE	ARG	A	704	16.360	84.323	22.247	1.00	1.34	A	N
ATOM	1407	CZ	ARG	A	704	16.705	83.462	21.297	1.00	2.98	A	C
ATOM	1408	NH1	ARG	A	704	17.853	82.816	21.386	1.00	3.22	A	N
ATOM	1409	NH2	ARG	A	704	15.904	83.239	20.263	1.00	2.29	A	N
ATOM	1410	C	ARG	A	704	18.270	89.115	23.403	1.00	6.00	A	C
ATOM	1411	O	ARG	A	704	19.056	89.337	24.329	1.00	6.23	A	O
ATOM	1412	N	GLU	A	705	17.641	90.080	22.719	1.00	8.87	A	N
ATOM	1413	CA	GLU	A	705	17.860	91.523	22.909	1.00	11.55	A	C
ATOM	1414	CB	GLU	A	705	17.050	92.084	24.087	1.00	9.59	A	C
ATOM	1415	CG	GLU	A	705	17.406	91.576	25.475	1.00	7.03	A	C
ATOM	1416	CD	GLU	A	705	16.345	91.955	26.532	1.00	5.39	A	C
ATOM	1417	OE1	GLU	A	705	16.531	91.602	27.726	1.00	4.32	A	O
ATOM	1418	OE2	GLU	A	705	15.322	92.599	26.170	1.00	3.90	A	O
ATOM	1419	C	GLU	A	705	19.346	91.819	23.065	1.00	13.29	A	C
ATOM	1420	O	GLU	A	705	20.179	91.052	22.575	1.00	14.70	A	O

ATOM	1421	N	GLY	A	706	19.698	92.928	23.711	1.00	14.58	A	N
ATOM	1422	CA	GLY	A	706	21.116	93.243	23.860	1.00	13.30	A	C
ATOM	1423	C	GLY	A	706	21.533	94.695	24.063	1.00	13.20	A	C
ATOM	1424	O	GLY	A	706	20.694	95.601	24.159	1.00	14.43	A	O
ATOM	1425	N	ASN	A	707	22.849	94.902	24.132	1.00	11.55	A	N
ATOM	1426	CA	ASN	A	707	23.463	96.221	24.335	1.00	9.56	A	C
ATOM	1427	CB	ASN	A	707	23.500	96.567	25.841	1.00	5.07	A	C
ATOM	1428	CG	ASN	A	707	23.740	98.063	26.123	1.00	1.03	A	C
ATOM	1429	OD1	ASN	A	707	23.426	98.548	27.213	1.00	0.00	A	O
ATOM	1430	ND2	ASN	A	707	24.299	98.782	25.158	1.00	0.00	A	N
ATOM	1431	C	ASN	A	707	24.877	96.042	23.821	1.00	10.04	A	C
ATOM	1432	O	ASN	A	707	25.588	95.198	24.334	1.00	9.41	A	O
ATOM	1433	N	SER	A	708	25.284	96.820	22.818	1.00	10.68	A	N
ATOM	1434	CA	SER	A	708	26.635	96.694	22.255	1.00	10.31	A	C
ATOM	1435	CB	SER	A	708	26.893	97.751	21.188	1.00	9.93	A	C
ATOM	1436	OG	SER	A	708	28.170	97.541	20.599	1.00	9.05	A	O
ATOM	1437	C	SER	A	708	27.780	96.738	23.262	1.00	10.39	A	C
ATOM	1438	O	SER	A	708	28.941	96.598	22.885	1.00	11.52	A	O
ATOM	1439	N	SER	A	709	27.467	96.974	24.532	1.00	9.40	A	N
ATOM	1440	CA	SER	A	709	28.494	96.957	25.569	1.00	8.56	A	C
ATOM	1441	CB	SER	A	709	28.253	98.053	26.618	1.00	5.99	A	C
ATOM	1442	OG	SER	A	709	28.697	99.320	26.147	1.00	1.95	A	O
ATOM	1443	C	SER	A	709	28.343	95.563	26.177	1.00	9.62	A	C
ATOM	1444	O	SER	A	709	29.295	94.987	26.711	1.00	8.59	A	O
ATOM	1445	N	GLN	A	710	27.125	95.032	26.048	1.00	11.06	A	N
ATOM	1446	CA	GLN	A	710	26.763	93.697	26.529	1.00	11.27	A	C
ATOM	1447	CB	GLN	A	710	25.417	93.758	27.288	1.00	10.72	A	C
ATOM	1448	CG	GLN	A	710	25.143	92.547	28.203	1.00	10.12	A	C
ATOM	1449	CD	GLN	A	710	23.981	92.749	29.175	1.00	9.53	A	C
ATOM	1450	OE1	GLN	A	710	24.084	93.502	30.146	1.00	8.92	A	O
ATOM	1451	NE2	GLN	A	710	22.871	92.068	28.912	1.00	8.68	A	N
ATOM	1452	C	GLN	A	710	26.698	92.735	25.313	1.00	10.93	A	C
ATOM	1453	O	GLN	A	710	26.680	91.499	25.458	1.00	11.13	A	O
ATOM	1454	N	ASN	A	711	26.665	93.312	24.114	1.00	9.97	A	N
ATOM	1455	CA	ASN	A	711	26.660	92.511	22.901	1.00	9.00	A	C
ATOM	1456	CB	ASN	A	711	26.429	93.369	21.645	1.00	9.76	A	C
ATOM	1457	CG	ASN	A	711	24.949	93.527	21.290	1.00	10.03	A	C
ATOM	1458	OD1	ASN	A	711	24.608	93.787	20.135	1.00	10.50	A	O
ATOM	1459	ND2	ASN	A	711	24.071	93.380	22.279	1.00	10.24	A	N
ATOM	1460	C	ASN	A	711	28.075	91.962	22.898	1.00	8.33	A	C
ATOM	1461	O	ASN	A	711	28.299	90.820	23.293	1.00	8.46	A	O
ATOM	1462	N	TRP	A	712	29.028	92.797	22.490	1.00	7.41	A	N
ATOM	1463	CA	TRP	A	712	30.431	92.405	22.459	1.00	6.17	A	C
ATOM	1464	CB	TRP	A	712	31.268	93.454	21.703	1.00	4.41	A	C
ATOM	1465	CG	TRP	A	712	31.288	93.276	20.202	1.00	2.75	A	C
ATOM	1466	CD2	TRP	A	712	30.725	94.153	19.223	1.00	1.92	A	C
ATOM	1467	CE2	TRP	A	712	30.982	93.581	17.949	1.00	1.81	A	C
ATOM	1468	CE3	TRP	A	712	30.029	95.369	19.295	1.00	2.80	A	C
ATOM	1469	CD1	TRP	A	712	31.848	92.240	19.503	1.00	1.53	A	C
ATOM	1470	NE1	TRP	A	712	31.670	92.417	18.151	1.00	0.68	A	N
ATOM	1471	CZ2	TRP	A	712	30.567	94.181	16.755	1.00	0.96	A	C
ATOM	1472	CZ3	TRP	A	712	29.614	95.978	18.102	1.00	3.24	A	C
ATOM	1473	CH2	TRP	A	712	29.888	95.377	16.846	1.00	2.47	A	C
ATOM	1474	C	TRP	A	712	30.966	92.228	23.887	1.00	6.22	A	C
ATOM	1475	O	TRP	A	712	32.105	92.587	24.175	1.00	7.16	A	O
ATOM	1476	N	GLN	A	713	30.136	91.673	24.770	1.00	6.28	A	N
ATOM	1477	CA	GLN	A	713	30.495	91.421	26.173	1.00	6.98	A	C
ATOM	1478	CB	GLN	A	713	29.628	92.292	27.096	1.00	6.75	A	C
ATOM	1479	CG	GLN	A	713	30.334	92.903	28.306	1.00	5.77	A	C
ATOM	1480	CD	GLN	A	713	30.793	91.879	29.328	1.00	4.57	A	C
ATOM	1481	OE1	GLN	A	713	31.801	91.199	29.144	1.00	1.74	A	O
ATOM	1482	NE2	GLN	A	713	30.045	91.764	30.413	1.00	3.96	A	N
ATOM	1483	C	GLN	A	713	30.259	89.919	26.469	1.00	7.67	A	C
ATOM	1484	O	GLN	A	713	30.728	89.368	27.484	1.00	6.98	A	O
ATOM	1485	N	ARG	A	714	29.506	89.270	25.581	1.00	7.37	A	N
ATOM	1486	CA	ARG	A	714	29.240	87.841	25.697	1.00	5.42	A	C
ATOM	1487	CB	ARG	A	714	27.742	87.525	25.585	1.00	6.30	A	C
ATOM	1488	CG	ARG	A	714	27.138	86.905	26.859	1.00	5.80	A	C
ATOM	1489	CD	ARG	A	714	25.671	86.566	26.686	1.00	4.97	A	C
ATOM	1490	NE	ARG	A	714	25.469	85.293	25.998	1.00	5.34	A	N
ATOM	1491	CZ	ARG	A	714	25.344	84.118	26.610	1.00	1.70	A	C
ATOM	1492	NH1	ARG	A	714	25.399	84.049	27.930	1.00	0.14	A	N
ATOM	1493	NH2	ARG	A	714	25.160	83.014	25.903	1.00	0.00	A	N
ATOM	1494	C	ARG	A	714	29.986	87.211	24.550	1.00	3.09	A	C
ATOM	1495	O	ARG	A	714	30.481	86.111	24.663	1.00	1.92	A	O
ATOM	1496	N	PHE	A	715	30.078	87.923	23.441	1.00	1.34	A	N
ATOM	1497	CA	PHE	A	715	30.805	87.394	22.312	1.00	1.36	A	C
ATOM	1498	CB	PHE	A	715	30.852	88.350	21.139	1.00	1.08	A	C
ATOM	1499	CG	PHE	A	715	31.662	87.832	19.998	1.00	0.00	A	C
ATOM	1500	CD1	PHE	A	715	31.075	87.070	19.005	1.00	0.00	A	C
ATOM	1501	CD2	PHE	A	715	33.026	88.098	19.921	1.00	0.00	A	C

ATOM	1502	CE1	PHE	A	715	31.832	86.585	17.946	1.00	0.00	A	C
ATOM	1503	CE2	PHE	A	715	33.791	87.616	18.867	1.00	0.00	A	C
ATOM	1504	CZ	PHE	A	715	33.193	86.862	17.877	1.00	0.00	A	C
ATOM	1505	C	PHE	A	715	32.215	87.167	22.756	1.00	2.81	A	C
ATOM	1506	O	PHE	A	715	33.003	86.584	22.032	1.00	2.78	A	O
ATOM	1507	N	TYR	A	716	32.559	87.670	23.932	1.00	4.94	A	N
ATOM	1508	CA	TYR	A	716	33.898	87.429	24.433	1.00	6.32	A	C
ATOM	1509	CB	TYR	A	716	34.315	88.441	25.491	1.00	4.84	A	C
ATOM	1510	CG	TYR	A	716	35.684	88.113	26.048	1.00	5.32	A	C
ATOM	1511	CD1	TYR	A	716	35.827	87.469	27.273	1.00	4.24	A	C
ATOM	1512	CE1	TYR	A	716	37.077	87.083	27.740	1.00	4.26	A	C
ATOM	1513	CD2	TYR	A	716	36.837	88.368	25.304	1.00	4.98	A	C
ATOM	1514	CE2	TYR	A	716	38.089	87.984	25.763	1.00	4.48	A	C
ATOM	1515	CZ	TYR	A	716	38.202	87.340	26.980	1.00	4.17	A	C
ATOM	1516	OH	TYR	A	716	39.440	86.943	27.435	1.00	5.02	A	O
ATOM	1517	C	TYR	A	716	33.851	86.049	25.063	1.00	6.65	A	C
ATOM	1518	O	TYR	A	716	34.599	85.151	24.677	1.00	7.40	A	C
ATOM	1519	N	GLN	A	717	32.946	85.884	26.023	1.00	5.38	A	N
ATOM	1520	CA	GLN	A	717	32.775	84.615	26.721	1.00	4.32	A	C
ATOM	1521	CB	GLN	A	717	31.696	84.775	27.786	1.00	4.38	A	C
ATOM	1522	CG	GLN	A	717	32.118	85.659	28.948	1.00	3.72	A	C
ATOM	1523	CD	GLN	A	717	33.157	84.985	29.807	1.00	3.02	A	C
ATOM	1524	OE1	GLN	A	717	33.586	85.522	30.823	1.00	0.12	A	O
ATOM	1525	NE2	GLN	A	717	33.569	83.787	29.401	1.00	3.65	A	N
ATOM	1526	C	GLN	A	717	32.463	83.420	25.811	1.00	3.42	A	C
ATOM	1527	O	GLN	A	717	33.073	82.363	25.957	1.00	1.69	A	O
ATOM	1528	N	LEU	A	718	31.524	83.578	24.881	1.00	3.14	A	N
ATOM	1529	CA	LEU	A	718	31.194	82.486	23.977	1.00	2.41	A	C
ATOM	1530	CB	LEU	A	718	29.994	82.815	23.097	1.00	1.83	A	C
ATOM	1531	CG	LEU	A	718	28.701	83.127	23.844	1.00	2.16	A	C
ATOM	1532	CD1	LEU	A	718	27.533	83.009	22.888	1.00	2.76	A	C
ATOM	1533	CD2	LEU	A	718	28.522	82.184	25.009	1.00	2.57	A	C
ATOM	1534	C	LEU	A	718	32.381	82.172	23.104	1.00	2.30	A	O
ATOM	1535	O	LEU	A	718	32.418	81.149	22.450	1.00	3.41	A	N
ATOM	1536	N	THR	A	719	33.352	83.065	23.069	1.00	2.24	A	C
ATOM	1537	CA	THR	A	719	34.549	82.795	22.293	1.00	3.59	A	C
ATOM	1538	CB	THR	A	719	35.034	84.083	21.532	1.00	4.42	A	C
ATOM	1539	OG1	THR	A	719	34.182	84.308	20.401	1.00	2.60	A	O
ATOM	1540	CG2	THR	A	719	36.471	83.941	21.028	1.00	3.27	A	C
ATOM	1541	C	THR	A	719	35.575	82.280	23.324	1.00	5.21	A	C
ATOM	1542	O	THR	A	719	36.647	81.780	22.976	1.00	4.34	A	O
ATOM	1543	N	LYS	A	720	35.193	82.379	24.600	1.00	6.41	A	N
ATOM	1544	CA	LYS	A	720	36.007	81.929	25.734	1.00	7.03	A	C
ATOM	1545	CB	LYS	A	720	35.539	82.619	27.025	1.00	6.13	A	C
ATOM	1546	CG	LYS	A	720	36.539	82.620	28.182	1.00	5.37	A	C
ATOM	1547	CD	LYS	A	720	37.663	83.634	27.977	1.00	3.60	A	C
ATOM	1548	CE	LYS	A	720	38.589	83.700	29.189	1.00	2.91	A	C
ATOM	1549	NZ	LYS	A	720	37.903	84.103	30.446	1.00	1.42	A	N
ATOM	1550	C	LYS	A	720	35.782	80.421	25.855	1.00	7.38	A	C
ATOM	1551	O	LYS	A	720	36.730	79.631	25.908	1.00	7.74	A	O
ATOM	1552	N	LEU	A	721	34.512	80.030	25.910	1.00	7.00	A	N
ATOM	1553	CA	LEU	A	721	34.169	78.619	25.992	1.00	7.12	A	C
ATOM	1554	CB	LEU	A	721	32.660	78.435	25.860	1.00	5.23	A	C
ATOM	1555	CG	LEU	A	721	32.169	77.021	26.130	1.00	4.81	A	C
ATOM	1556	CD1	LEU	A	721	32.511	76.597	27.548	1.00	4.72	A	C
ATOM	1557	CD2	LEU	A	721	30.695	76.983	25.916	1.00	4.28	A	C
ATOM	1558	C	LEU	A	721	34.885	77.924	24.836	1.00	7.81	A	C
ATOM	1559	O	LEU	A	721	35.878	77.237	25.040	1.00	5.88	A	O
ATOM	1560	N	LEU	A	722	34.385	78.126	23.621	1.00	7.41	A	N
ATOM	1561	CA	LEU	A	722	34.994	77.537	22.431	1.00	4.26	A	C
ATOM	1562	CB	LEU	A	722	34.457	78.159	21.142	1.00	2.07	A	C
ATOM	1563	CG	LEU	A	722	33.007	77.983	20.721	1.00	1.49	A	C
ATOM	1564	CD1	LEU	A	722	32.762	78.829	19.508	1.00	1.51	A	C
ATOM	1565	CD2	LEU	A	722	32.723	76.537	20.414	1.00	0.89	A	C
ATOM	1566	C	LEU	A	722	36.474	77.783	22.456	1.00	1.91	A	C
ATOM	1567	O	LEU	A	722	37.200	77.226	21.649	1.00	4.15	A	O
ATOM	1568	N	ASP	A	723	36.922	78.654	23.348	1.00	0.00	A	N
ATOM	1569	CA	ASP	A	723	38.341	78.930	23.444	1.00	0.00	A	C
ATOM	1570	CB	ASP	A	723	38.577	80.320	24.012	1.00	2.77	A	C
ATOM	1571	CG	ASP	A	723	39.382	81.181	23.085	1.00	1.89	A	C
ATOM	1572	OD1	ASP	A	723	39.076	81.134	21.875	1.00	1.94	A	O
ATOM	1573	OD2	ASP	A	723	40.304	81.892	23.562	1.00	2.67	A	O
ATOM	1574	C	ASP	A	723	38.927	77.893	24.361	1.00	0.07	A	C
ATOM	1575	O	ASP	A	723	39.994	77.352	24.080	1.00	0.00	A	O
ATOM	1576	N	SER	A	724	38.207	77.625	25.452	1.00	0.04	A	N
ATOM	1577	CA	SER	A	724	38.602	76.632	26.446	1.00	0.49	A	C
ATOM	1578	CB	SER	A	724	37.863	76.858	27.768	1.00	0.00	A	C
ATOM	1579	OG	SER	A	724	36.479	76.578	27.646	1.00	0.00	A	O
ATOM	1580	C	SER	A	724	38.286	75.233	25.927	1.00	0.77	A	C
ATOM	1581	O	SER	A	724	38.554	74.239	26.593	1.00	0.00	A	O
ATOM	1582	N	MET	A	725	37.717	75.160	24.730	1.00	1.57	A	N

ATOM	1583	CA	MET	A	725	37.386	73.878	24.142	1.00	3.27	A	C
ATOM	1584	CB	MET	A	725	36.446	74.057	22.955	1.00	1.49	A	C
ATOM	1585	CG	MET	A	725	35.003	74.115	23.378	1.00	0.00	A	C
ATOM	1586	SD	MET	A	725	34.593	72.720	24.435	1.00	0.00	A	S
ATOM	1587	CE	MET	A	725	34.143	71.571	23.228	1.00	0.00	A	C
ATOM	1588	C	MET	A	725	38.598	73.071	23.723	1.00	5.34	A	C
ATOM	1589	O	MET	A	725	38.750	71.922	24.142	1.00	6.48	A	O
ATOM	1590	N	HIS	A	726	39.466	73.659	22.904	1.00	6.92	A	N
ATOM	1591	CA	HIS	A	726	40.661	72.940	22.450	1.00	7.76	A	C
ATOM	1592	CB	HIS	A	726	41.604	73.870	21.699	1.00	7.20	A	C
ATOM	1593	CG	HIS	A	726	40.914	74.821	20.771	1.00	8.49	A	C
ATOM	1594	CD2	HIS	A	726	41.087	75.054	19.449	1.00	7.36	A	C
ATOM	1595	ND1	HIS	A	726	39.970	75.726	21.202	1.00	6.69	A	N
ATOM	1596	CE1	HIS	A	726	39.594	76.480	20.184	1.00	7.19	A	C
ATOM	1597	NE2	HIS	A	726	40.258	76.093	19.110	1.00	7.57	A	N
ATOM	1598	C	HIS	A	726	41.409	72.340	23.639	1.00	7.38	A	C
ATOM	1599	O	HIS	A	726	41.919	71.225	23.558	1.00	7.19	A	O
ATOM	1600	N	GLU	A	727	41.477	73.089	24.737	1.00	6.23	A	N
ATOM	1601	CA	GLU	A	727	42.156	72.622	25.938	1.00	4.21	A	C
ATOM	1602	CB	GLU	A	727	42.345	73.779	26.942	1.00	6.03	A	C
ATOM	1603	CG	GLU	A	727	43.378	74.844	26.524	1.00	8.05	A	C
ATOM	1604	CD	GLU	A	727	44.452	75.125	27.606	1.00	9.58	A	C
ATOM	1605	OE1	GLU	A	727	44.079	75.498	28.743	1.00	10.35	A	O
ATOM	1606	OE2	GLU	A	727	45.670	74.975	27.318	1.00	9.03	A	O
ATOM	1607	C	GLU	A	727	41.406	71.475	26.615	1.00	1.78	A	C
ATOM	1608	O	GLU	A	727	41.932	70.845	27.512	1.00	2.34	A	O
ATOM	1609	N	VAL	A	728	40.182	71.200	26.186	1.00	0.00	A	N
ATOM	1610	CA	VAL	A	728	39.388	70.133	26.795	1.00	0.00	A	C
ATOM	1611	CB	VAL	A	728	37.862	70.430	26.686	1.00	0.00	A	C
ATOM	1612	CG1	VAL	A	728	37.066	69.203	27.041	1.00	0.00	A	C
ATOM	1613	CG2	VAL	A	728	37.473	71.574	27.618	1.00	0.00	A	C
ATOM	1614	C	VAL	A	728	39.659	68.795	26.131	1.00	0.00	A	C
ATOM	1615	O	VAL	A	728	40.085	67.841	26.770	1.00	0.00	A	O
ATOM	1616	N	VAL	A	729	39.398	68.749	24.834	1.00	0.98	A	N
ATOM	1617	CA	VAL	A	729	39.578	67.564	24.016	1.00	1.12	A	C
ATOM	1618	CB	VAL	A	729	39.193	67.888	22.572	1.00	0.91	A	C
ATOM	1619	CG1	VAL	A	729	39.412	66.717	21.689	1.00	0.99	A	C
ATOM	1620	CG2	VAL	A	729	37.748	68.296	22.527	1.00	3.41	A	C
ATOM	1621	C	VAL	A	729	40.969	66.933	24.063	1.00	0.04	A	C
ATOM	1622	O	VAL	A	729	41.113	65.766	23.742	1.00	0.54	A	O
ATOM	1623	N	GLU	A	730	41.997	67.684	24.445	1.00	0.00	A	N
ATOM	1624	CA	GLU	A	730	43.317	67.078	24.539	1.00	0.00	A	C
ATOM	1625	CB	GLU	A	730	44.418	68.111	24.814	1.00	0.00	A	C
ATOM	1626	CG	GLU	A	730	45.869	67.518	24.894	1.00	0.00	A	C
ATOM	1627	CD	GLU	A	730	46.540	67.685	26.272	1.00	0.00	A	C
ATOM	1628	OE1	GLU	A	730	47.701	67.266	26.422	1.00	0.00	A	O
ATOM	1629	OE2	GLU	A	730	45.913	68.231	27.211	1.00	0.08	A	O
ATOM	1630	C	GLU	A	730	43.209	66.153	25.726	1.00	0.00	A	C
ATOM	1631	O	GLU	A	730	43.744	65.046	25.716	1.00	0.00	A	O
ATOM	1632	N	ASN	A	731	42.510	66.619	26.755	1.00	0.00	A	N
ATOM	1633	CA	ASN	A	731	42.317	65.824	27.963	1.00	0.00	A	C
ATOM	1634	CB	ASN	A	731	41.755	66.694	29.086	1.00	0.00	A	C
ATOM	1635	CG	ASN	A	731	42.811	67.545	29.731	1.00	0.00	A	C
ATOM	1636	OD1	ASN	A	731	42.736	67.829	30.924	1.00	0.00	A	O
ATOM	1637	ND2	ASN	A	731	43.810	67.962	28.949	1.00	0.00	A	N
ATOM	1638	C	ASN	A	731	41.411	64.609	27.748	1.00	0.00	A	C
ATOM	1639	O	ASN	A	731	41.661	63.521	28.273	1.00	0.00	A	O
ATOM	1640	N	LEU	A	732	40.352	64.806	26.979	1.00	0.00	A	N
ATOM	1641	CA	LEU	A	732	39.430	63.739	26.695	1.00	0.00	A	C
ATOM	1642	CB	LEU	A	732	38.126	64.329	26.178	1.00	0.00	A	C
ATOM	1643	CG	LEU	A	732	37.030	64.595	27.207	1.00	0.00	A	C
ATOM	1644	CD1	LEU	A	732	36.288	63.300	27.408	1.00	0.00	A	C
ATOM	1645	CD2	LEU	A	732	37.594	65.116	28.515	1.00	0.00	A	C
ATOM	1646	C	LEU	A	732	40.049	62.800	25.682	1.00	0.00	A	C
ATOM	1647	O	LEU	A	732	40.056	61.594	25.889	1.00	0.00	A	O
ATOM	1648	N	LEU	A	733	40.574	63.341	24.586	1.00	0.00	A	N
ATOM	1649	CA	LEU	A	733	41.225	62.502	23.571	1.00	0.26	A	C
ATOM	1650	CB	LEU	A	733	41.862	63.353	22.475	1.00	0.03	A	C
ATOM	1651	CG	LEU	A	733	40.887	64.176	21.641	1.00	1.12	A	C
ATOM	1652	CD1	LEU	A	733	41.638	64.855	20.492	1.00	1.37	A	C
ATOM	1653	CD2	LEU	A	733	39.767	63.262	21.133	1.00	3.49	A	C
ATOM	1654	C	LEU	A	733	42.310	61.659	24.225	1.00	0.77	A	C
ATOM	1655	O	LEU	A	733	42.451	60.480	23.942	1.00	0.00	A	O
ATOM	1656	N	ASN	A	734	43.078	62.296	25.101	1.00	1.40	A	N
ATOM	1657	CA	ASN	A	734	44.136	61.637	25.843	1.00	2.49	A	C
ATOM	1658	CB	ASN	A	734	44.876	62.659	26.723	1.00	1.09	A	C
ATOM	1659	CG	ASN	A	734	46.027	63.343	26.003	1.00	1.78	A	C
ATOM	1660	OD1	ASN	A	734	45.954	63.633	24.811	1.00	1.62	A	O
ATOM	1661	ND2	ASN	A	734	47.095	63.611	26.739	1.00	0.97	A	N
ATOM	1662	C	ASN	A	734	43.510	60.563	26.725	1.00	3.73	A	C
ATOM	1663	O	ASN	A	734	44.080	60.192	27.738	1.00	5.37	A	O

ATOM	1664	N	TYR	A	735	42.329	60.084	26.351	1.00	5.64	A	N
ATOM	1665	CA	TYR	A	735	41.646	59.041	27.115	1.00	7.62	A	C
ATOM	1666	CB	TYR	A	735	40.944	59.651	28.342	1.00	7.88	A	C
ATOM	1667	CG	TYR	A	735	41.295	59.013	29.687	1.00	8.63	A	C
ATOM	1668	CD1	TYR	A	735	41.092	57.650	29.912	1.00	8.27	A	C
ATOM	1669	CE1	TYR	A	735	41.369	57.069	31.158	1.00	7.44	A	C
ATOM	1670	CD2	TYR	A	735	41.789	59.785	30.746	1.00	7.71	A	C
ATOM	1671	CE2	TYR	A	735	42.069	59.217	31.996	1.00	6.69	A	C
ATOM	1672	CZ	TYR	A	735	41.858	57.853	32.196	1.00	7.17	A	C
ATOM	1673	OH	TYR	A	735	42.151	57.261	33.413	1.00	6.25	A	O
ATOM	1674	C	TYR	A	735	40.636	58.275	26.231	1.00	8.33	A	C
ATOM	1675	O	TYR	A	735	39.890	57.417	26.706	1.00	9.28	A	O
ATOM	1676	N	CYS	A	736	40.603	58.607	24.947	1.00	8.05	A	N
ATOM	1677	CA	CYS	A	736	39.736	57.926	23.992	1.00	7.40	A	C
ATOM	1678	CB	CYS	A	736	38.700	58.899	23.409	1.00	7.12	A	C
ATOM	1679	SG	CYS	A	736	39.325	60.290	22.421	1.00	5.81	A	S
ATOM	1680	C	CYS	A	736	40.727	57.485	22.933	1.00	7.61	A	C
ATOM	1681	O	CYS	A	736	40.403	56.833	21.952	1.00	8.89	A	O
ATOM	1682	N	PHE	A	737	41.961	57.883	23.196	1.00	7.54	A	N
ATOM	1683	CA	PHE	A	737	43.154	57.632	22.398	1.00	6.57	A	C
ATOM	1684	CB	PHE	A	737	43.849	58.978	22.140	1.00	5.79	A	C
ATOM	1685	CG	PHE	A	737	45.230	58.871	21.572	1.00	3.18	A	C
ATOM	1686	CD1	PHE	A	737	45.441	58.945	20.203	1.00	3.63	A	C
ATOM	1687	CD2	PHE	A	737	46.319	58.728	22.403	1.00	2.19	A	C
ATOM	1688	CE1	PHE	A	737	46.721	58.879	19.673	1.00	0.91	A	C
ATOM	1689	CE2	PHE	A	737	47.599	58.661	21.882	1.00	2.56	A	C
ATOM	1690	CZ	PHE	A	737	47.800	58.738	20.516	1.00	1.43	A	C
ATOM	1691	C	PHE	A	737	44.005	56.771	23.333	1.00	6.49	A	C
ATOM	1692	O	PHE	A	737	44.808	55.951	22.899	1.00	6.32	A	O
ATOM	1693	N	GLN	A	738	43.795	56.982	24.628	1.00	6.22	A	N
ATOM	1694	CA	GLN	A	738	44.498	56.275	25.677	1.00	6.20	A	C
ATOM	1695	CB	GLN	A	738	45.355	57.266	26.455	1.00	6.44	A	C
ATOM	1696	CG	GLN	A	738	46.147	56.669	27.606	1.00	8.72	A	C
ATOM	1697	CD	GLN	A	738	46.808	57.738	28.468	1.00	9.91	A	C
ATOM	1698	OE1	GLN	A	738	47.444	58.667	27.945	1.00	9.37	A	O
ATOM	1699	NE2	GLN	A	738	46.666	57.612	29.796	1.00	9.20	A	N
ATOM	1700	C	GLN	A	738	43.496	55.608	26.612	1.00	6.57	A	C
ATOM	1701	O	GLN	A	738	9999.0009999	9999.0009999	9999.000	1.00	0.00	A	O
ATOM	1702	OXT	GLN	A	738	9999.0009999	9999.0009999	9999.000	1.00	0.00	A	O
ATOM	1703	CB	THR	B	531	16.410	64.698	54.095	1.00	10.97	B	C
ATOM	1704	OG1	THR	B	531	16.356	64.023	52.823	1.00	11.15	B	O
ATOM	1705	CG2	THR	B	531	15.335	65.780	54.147	1.00	10.76	B	C
ATOM	1706	C	THR	B	531	18.864	64.287	54.076	1.00	9.19	B	C
ATOM	1707	O	THR	B	531	19.150	63.911	52.942	1.00	9.20	B	O
ATOM	1708	N	THR	B	531	18.022	66.485	53.369	1.00	9.74	B	N
ATOM	1709	CA	THR	B	531	17.801	65.342	54.305	1.00	10.21	B	C
ATOM	1710	N	LEU	B	532	19.468	63.820	55.155	1.00	7.92	B	N
ATOM	1711	CA	LEU	B	532	20.491	62.803	55.027	1.00	8.18	B	C
ATOM	1712	CB	LEU	B	532	21.857	63.445	54.782	1.00	10.08	B	C
ATOM	1713	CG	LEU	B	532	22.989	62.475	54.431	1.00	11.85	B	C
ATOM	1714	CD1	LEU	B	532	24.127	63.239	53.767	1.00	12.62	B	C
ATOM	1715	CD2	LEU	B	532	23.459	61.751	55.688	1.00	12.93	B	C
ATOM	1716	C	LEU	B	532	20.520	61.935	56.267	1.00	7.59	B	C
ATOM	1717	O	LEU	B	532	20.734	60.730	56.181	1.00	6.51	B	O
ATOM	1718	N	VAL	B	533	20.305	62.550	57.422	1.00	7.14	B	N
ATOM	1719	CA	VAL	B	533	20.290	61.799	58.654	1.00	5.56	B	C
ATOM	1720	CB	VAL	B	533	20.100	62.714	59.865	1.00	2.34	B	C
ATOM	1721	CG1	VAL	B	533	20.199	61.925	61.137	1.00	0.89	B	C
ATOM	1722	CG2	VAL	B	533	21.168	63.777	59.860	1.00	0.44	B	C
ATOM	1723	C	VAL	B	533	19.132	60.822	58.541	1.00	6.57	B	C
ATOM	1724	O	VAL	B	533	19.148	59.758	59.168	1.00	6.85	B	O
ATOM	1725	N	SER	B	534	18.140	61.164	57.716	1.00	6.99	B	N
ATOM	1726	CA	SER	B	534	16.984	60.284	57.519	1.00	6.87	B	C
ATOM	1727	CB	SER	B	534	15.873	61.009	56.766	1.00	4.90	B	C
ATOM	1728	OG	SER	B	534	15.270	61.978	57.598	1.00	2.12	B	O
ATOM	1729	C	SER	B	534	17.347	58.995	56.780	1.00	7.24	B	C
ATOM	1730	O	SER	B	534	17.177	57.896	57.320	1.00	6.08	B	O
ATOM	1731	N	LEU	B	535	17.842	59.116	55.551	1.00	7.19	B	N
ATOM	1732	CA	LEU	B	535	18.221	57.914	54.831	1.00	7.23	B	C
ATOM	1733	CB	LEU	B	535	18.816	58.234	53.452	1.00	7.69	B	C
ATOM	1734	CG	LEU	B	535	20.061	59.095	53.258	1.00	8.04	B	C
ATOM	1735	CD1	LEU	B	535	20.773	58.693	51.957	1.00	7.50	B	C
ATOM	1736	CD2	LEU	B	535	19.656	60.546	53.224	1.00	6.73	B	C
ATOM	1737	C	LEU	B	535	19.225	57.159	55.698	1.00	7.12	B	C
ATOM	1738	O	LEU	B	535	19.299	55.930	55.660	1.00	6.71	B	O
ATOM	1739	N	LEU	B	536	19.998	57.899	56.484	1.00	7.30	B	N
ATOM	1740	CA	LEU	B	536	20.942	57.265	57.391	1.00	6.15	B	C
ATOM	1741	CB	LEU	B	536	21.789	58.292	58.145	1.00	2.76	B	C
ATOM	1742	CG	LEU	B	536	23.077	58.872	57.571	1.00	0.00	B	C
ATOM	1743	CD1	LEU	B	536	23.709	59.740	58.652	1.00	0.00	B	C
ATOM	1744	CD2	LEU	B	536	24.030	57.779	57.159	1.00	0.00	B	C

ATOM	1745	C	LEU	B	536	20.108	56.496	58.412	1.00	6.88	B	C
ATOM	1746	O	LEU	B	536	20.263	55.287	58.574	1.00	7.30	B	O
ATOM	1747	N	GLU	B	537	19.211	57.203	59.091	1.00	6.66	B	N
ATOM	1748	CA	GLU	B	537	18.382	56.562	60.099	1.00	7.24	B	C
ATOM	1749	CB	GLU	B	537	17.321	57.536	60.636	1.00	7.42	B	C
ATOM	1750	CG	GLU	B	537	16.561	56.956	61.836	1.00	4.99	B	C
ATOM	1751	CD	GLU	B	537	15.238	57.632	62.131	1.00	3.13	B	C
ATOM	1752	OE1	GLU	B	537	15.251	58.728	62.729	1.00	1.34	B	O
ATOM	1753	OE2	GLU	B	537	14.187	57.058	61.767	1.00	3.54	B	O
ATOM	1754	C	GLU	B	537	17.683	55.273	59.621	1.00	7.55	B	C
ATOM	1755	O	GLU	B	537	17.593	54.295	60.376	1.00	7.59	B	O
ATOM	1756	N	VAL	B	538	17.201	55.269	58.377	1.00	6.83	B	N
ATOM	1757	CA	VAL	B	538	16.481	54.117	57.831	1.00	5.38	B	C
ATOM	1758	CB	VAL	B	538	15.534	54.577	56.700	1.00	5.91	B	C
ATOM	1759	CG1	VAL	B	538	14.862	53.378	56.058	1.00	3.94	B	C
ATOM	1760	CG2	VAL	B	538	14.477	55.541	57.270	1.00	5.56	B	C
ATOM	1761	C	VAL	B	538	17.341	52.941	57.350	1.00	4.64	B	C
ATOM	1762	O	VAL	B	538	16.838	51.846	57.126	1.00	2.68	B	O
ATOM	1763	N	ILE	B	539	18.639	53.171	57.188	1.00	5.06	B	N
ATOM	1764	CA	ILE	B	539	19.559	52.105	56.785	1.00	5.67	B	C
ATOM	1765	CB	ILE	B	539	20.529	52.536	55.646	1.00	6.10	B	C
ATOM	1766	CG2	ILE	B	539	19.744	52.930	54.416	1.00	6.78	B	C
ATOM	1767	CG1	ILE	B	539	21.426	53.682	56.111	1.00	3.64	B	C
ATOM	1768	CD1	ILE	B	539	22.485	54.029	55.119	1.00	0.00	B	C
ATOM	1769	C	ILE	B	539	20.397	51.735	58.006	1.00	5.53	B	C
ATOM	1770	O	ILE	B	539	21.570	51.392	57.899	1.00	6.20	B	O
ATOM	1771	N	GLU	B	540	19.779	51.838	59.173	1.00	5.03	B	N
ATOM	1772	CA	GLU	B	540	20.441	51.511	60.417	1.00	5.17	B	C
ATOM	1773	CB	GLU	B	540	20.053	52.521	61.495	1.00	6.83	B	C
ATOM	1774	CG	GLU	B	540	21.225	53.264	62.103	1.00	10.34	B	C
ATOM	1775	CD	GLU	B	540	21.970	54.107	61.093	1.00	11.52	B	C
ATOM	1776	OE1	GLU	B	540	22.905	54.838	61.491	1.00	12.12	B	O
ATOM	1777	OE2	GLU	B	540	21.621	54.034	59.899	1.00	12.58	B	O
ATOM	1778	C	GLU	B	540	19.981	50.113	60.816	1.00	4.17	B	C
ATOM	1779	O	GLU	B	540	19.001	49.964	61.542	1.00	3.92	B	O
ATOM	1780	N	PRO	B	541	20.687	49.071	60.341	1.00	3.62	B	N
ATOM	1781	CD	PRO	B	541	22.029	49.119	59.725	1.00	3.05	B	C
ATOM	1782	CA	PRO	B	541	20.330	47.694	60.660	1.00	2.38	B	C
ATOM	1783	CB	PRO	B	541	21.687	47.005	60.651	1.00	2.74	B	C
ATOM	1784	CG	PRO	B	541	22.346	47.659	59.491	1.00	2.55	B	C
ATOM	1785	C	PRO	B	541	19.592	47.576	61.986	1.00	1.31	B	C
ATOM	1786	O	PRO	B	541	19.919	48.273	62.943	1.00	0.84	B	O
ATOM	1787	N	GLU	B	542	18.595	46.694	62.031	1.00	0.24	B	N
ATOM	1788	CA	GLU	B	542	17.793	46.501	63.235	1.00	1.23	B	C
ATOM	1789	CB	GLU	B	542	16.327	46.202	62.859	1.00	2.38	B	C
ATOM	1790	CG	GLU	B	542	15.260	46.947	63.711	1.00	4.01	B	C
ATOM	1791	CD	GLU	B	542	13.815	46.670	63.257	1.00	3.74	B	C
ATOM	1792	OE1	GLU	B	542	13.541	46.787	62.044	1.00	4.61	B	O
ATOM	1793	OE2	GLU	B	542	12.953	46.346	64.109	1.00	2.28	B	O
ATOM	1794	C	GLU	B	542	18.322	45.402	64.153	1.00	2.07	B	C
ATOM	1795	O	GLU	B	542	18.720	44.335	63.707	1.00	1.60	B	O
ATOM	1796	N	VAL	B	543	18.333	45.709	65.443	1.00	3.47	B	N
ATOM	1797	CA	VAL	B	543	18.758	44.810	66.506	1.00	3.43	B	C
ATOM	1798	CB	VAL	B	543	17.682	44.772	67.610	1.00	2.75	B	C
ATOM	1799	CG1	VAL	B	543	17.530	46.138	68.249	1.00	3.84	B	C
ATOM	1800	CG2	VAL	B	543	16.345	44.374	67.007	1.00	3.15	B	C
ATOM	1801	C	VAL	B	543	19.005	43.374	66.076	1.00	3.09	B	C
ATOM	1802	O	VAL	B	543	18.080	42.696	65.650	1.00	3.18	B	O
ATOM	1803	N	LEU	B	544	20.249	42.913	66.182	1.00	2.08	B	N
ATOM	1804	CA	LEU	B	544	20.575	41.532	65.840	1.00	2.37	B	C
ATOM	1805	CB	LEU	B	544	22.088	41.310	65.723	1.00	3.93	B	C
ATOM	1806	CG	LEU	B	544	22.866	41.683	64.454	1.00	5.41	B	C
ATOM	1807	CD1	LEU	B	544	24.257	41.083	64.523	1.00	4.85	B	C
ATOM	1808	CD2	LEU	B	544	22.164	41.155	63.225	1.00	6.58	B	C
ATOM	1809	C	LEU	B	544	20.050	40.704	66.994	1.00	2.40	B	C
ATOM	1810	O	LEU	B	544	20.542	40.808	68.118	1.00	0.97	B	O
ATOM	1811	N	TYR	B	545	19.031	39.896	66.721	1.00	3.79	B	N
ATOM	1812	CA	TYR	B	545	18.443	39.056	67.763	1.00	2.80	B	C
ATOM	1813	CB	TYR	B	545	16.994	38.659	67.421	1.00	0.40	B	C
ATOM	1814	CG	TYR	B	545	15.969	39.309	68.325	1.00	0.00	B	C
ATOM	1815	CD1	TYR	B	545	15.987	39.099	69.699	1.00	0.00	B	C
ATOM	1816	CE1	TYR	B	545	15.028	39.718	70.548	1.00	0.00	B	C
ATOM	1817	CD2	TYR	B	545	14.980	40.151	67.807	1.00	0.00	B	C
ATOM	1818	CE2	TYR	B	545	14.019	40.775	68.643	1.00	0.00	B	C
ATOM	1819	CZ	TYR	B	545	14.050	40.549	70.003	1.00	0.00	B	C
ATOM	1820	OH	TYR	B	545	13.091	41.106	70.804	1.00	0.00	B	O
ATOM	1821	C	TYR	B	545	19.332	37.836	67.895	1.00	3.58	B	C
ATOM	1822	O	TYR	B	545	19.282	36.911	67.080	1.00	3.31	B	O
ATOM	1823	N	ALA	B	546	20.174	37.864	68.921	1.00	3.29	B	N
ATOM	1824	CA	ALA	B	546	21.086	36.773	69.151	1.00	4.97	B	C
ATOM	1825	CB	ALA	B	546	22.046	37.122	70.272	1.00	5.14	B	C

ATOM	1826	C	ALA	B	546	20.298	35.516	69.482	1.00	5.45	B	C
ATOM	1827	O	ALA	B	546	19.819	34.815	68.580	1.00	5.06	B	O
ATOM	1828	N	GLY	B	547	20.149	35.244	70.772	1.00	5.37	B	N
ATOM	1829	CA	GLY	B	547	19.432	34.060	71.190	1.00	5.08	B	C
ATOM	1830	C	GLY	B	547	20.316	33.339	72.161	1.00	4.07	B	C
ATOM	1831	O	GLY	B	547	21.087	32.474	71.781	1.00	2.80	B	O
ATOM	1832	N	TYR	B	548	20.214	33.731	73.421	1.00	5.82	B	N
ATOM	1833	CA	TYR	B	548	21.013	33.143	74.478	1.00	7.20	B	C
ATOM	1834	CB	TYR	B	548	21.259	34.175	75.574	1.00	7.73	B	C
ATOM	1835	CG	TYR	B	548	22.370	33.825	76.535	1.00	8.10	B	C
ATOM	1836	CD1	TYR	B	548	22.171	33.910	77.910	1.00	7.45	B	C
ATOM	1837	CE1	TYR	B	548	23.206	33.662	78.800	1.00	7.36	B	C
ATOM	1838	CD2	TYR	B	548	23.639	33.474	76.073	1.00	7.72	B	C
ATOM	1839	CE2	TYR	B	548	24.681	33.225	76.958	1.00	6.30	B	C
ATOM	1840	CZ	TYR	B	548	24.454	33.323	78.317	1.00	6.72	B	C
ATOM	1841	OH	TYR	B	548	25.472	33.093	79.204	1.00	5.53	B	O
ATOM	1842	C	TYR	B	548	20.228	31.973	75.037	1.00	7.93	B	C
ATOM	1843	O	TYR	B	548	19.011	32.070	75.225	1.00	8.67	B	O
ATOM	1844	N	ASP	B	549	20.921	30.867	75.290	1.00	7.52	B	N
ATOM	1845	CA	ASP	B	549	20.269	29.677	75.813	1.00	6.89	B	C
ATOM	1846	CB	ASP	B	549	21.308	28.656	76.292	1.00	7.66	B	C
ATOM	1847	CG	ASP	B	549	22.073	27.999	75.139	1.00	6.01	B	C
ATOM	1848	OD1	ASP	B	549	23.125	27.385	75.407	1.00	4.80	B	O
ATOM	1849	OD2	ASP	B	549	21.623	28.086	73.976	1.00	6.15	B	O
ATOM	1850	C	ASP	B	549	19.396	30.113	76.956	1.00	6.54	B	C
ATOM	1851	O	ASP	B	549	18.253	29.684	77.067	1.00	5.87	B	O
ATOM	1852	N	SER	B	550	19.953	30.986	77.792	1.00	7.16	B	N
ATOM	1853	CA	SER	B	550	19.252	31.542	78.957	1.00	8.36	B	C
ATOM	1854	CB	SER	B	550	18.098	32.442	78.482	1.00	9.58	B	C
ATOM	1855	OG	SER	B	550	18.452	33.176	77.320	1.00	10.64	B	O
ATOM	1856	C	SER	B	550	18.701	30.439	79.887	1.00	8.38	B	C
ATOM	1857	O	SER	B	550	17.636	30.577	80.498	1.00	7.63	B	O
ATOM	1858	N	SER	B	551	19.445	29.348	79.991	1.00	8.02	B	N
ATOM	1859	CA	SER	B	551	19.029	28.227	80.808	1.00	7.30	B	C
ATOM	1860	CB	SER	B	551	18.385	27.153	79.907	1.00	7.81	B	C
ATOM	1861	OG	SER	B	551	17.257	27.649	79.197	1.00	7.28	B	O
ATOM	1862	C	SER	B	551	20.230	27.654	81.573	1.00	6.56	B	C
ATOM	1863	O	SER	B	551	20.089	27.165	82.696	1.00	6.94	B	O
ATOM	1864	N	VAL	B	552	21.405	27.721	80.950	1.00	5.24	B	N
ATOM	1865	CA	VAL	B	552	22.650	27.231	81.540	1.00	4.44	B	C
ATOM	1866	CB	VAL	B	552	23.646	26.778	80.438	1.00	3.65	B	C
ATOM	1867	CG1	VAL	B	552	24.553	25.672	80.968	1.00	1.31	B	C
ATOM	1868	CG2	VAL	B	552	22.886	26.314	79.203	1.00	2.44	B	C
ATOM	1869	C	VAL	B	552	23.279	28.392	82.318	1.00	4.09	B	C
ATOM	1870	O	VAL	B	552	23.518	29.463	81.745	1.00	4.59	B	O
ATOM	1871	N	PRO	B	553	23.574	28.198	83.621	1.00	3.98	B	N
ATOM	1872	CD	PRO	B	553	23.745	26.914	84.323	1.00	3.81	B	C
ATOM	1873	CA	PRO	B	553	24.171	29.289	84.398	1.00	4.58	B	C
ATOM	1874	CB	PRO	B	553	24.828	28.564	85.566	1.00	5.21	B	C
ATOM	1875	CG	PRO	B	553	23.972	27.358	85.744	1.00	3.58	B	C
ATOM	1876	C	PRO	B	553	25.177	30.014	83.513	1.00	5.01	B	C
ATOM	1877	O	PRO	B	553	25.828	29.393	82.672	1.00	6.50	B	O
ATOM	1878	N	ASP	B	554	25.309	31.320	83.692	1.00	5.82	B	N
ATOM	1879	CA	ASP	B	554	26.205	32.083	82.839	1.00	7.79	B	C
ATOM	1880	CB	ASP	B	554	26.000	33.586	83.044	1.00	10.98	B	C
ATOM	1881	CG	ASP	B	554	25.733	34.316	81.734	1.00	11.80	B	C
ATOM	1882	OD1	ASP	B	554	26.552	34.158	80.803	1.00	13.14	B	O
ATOM	1883	OD2	ASP	B	554	24.710	35.039	81.639	1.00	12.43	B	O
ATOM	1884	C	ASP	B	554	27.675	31.747	82.964	1.00	7.81	B	C
ATOM	1885	O	ASP	B	554	28.431	32.417	83.668	1.00	8.13	B	O
ATOM	1886	N	SER	B	555	28.069	30.696	82.257	1.00	7.82	B	N
ATOM	1887	CA	SER	B	555	29.448	30.252	82.232	1.00	7.61	B	C
ATOM	1888	CB	SER	B	555	29.507	28.794	81.782	1.00	5.61	B	C
ATOM	1889	OG	SER	B	555	28.828	28.617	80.555	1.00	2.11	B	O
ATOM	1890	C	SER	B	555	30.224	31.156	81.260	1.00	8.63	B	C
ATOM	1891	O	SER	B	555	29.946	31.199	80.051	1.00	7.85	B	O
ATOM	1892	N	THR	B	556	31.185	31.888	81.820	1.00	8.68	B	N
ATOM	1893	CA	THR	B	556	32.040	32.825	81.091	1.00	7.13	B	C
ATOM	1894	CB	THR	B	556	33.186	33.309	82.011	1.00	6.02	B	C
ATOM	1895	OG1	THR	B	556	34.346	33.616	81.230	1.00	6.08	B	O
ATOM	1896	CG2	THR	B	556	33.538	32.225	83.030	1.00	7.18	B	C
ATOM	1897	C	THR	B	556	32.626	32.311	79.769	1.00	6.09	B	C
ATOM	1898	O	THR	B	556	33.458	32.974	79.160	1.00	6.37	B	O
ATOM	1899	N	TRP	B	557	32.221	31.124	79.335	1.00	4.91	B	N
ATOM	1900	CA	TRP	B	557	32.702	30.603	78.060	1.00	4.54	B	C
ATOM	1901	CB	TRP	B	557	33.181	29.139	78.164	1.00	4.26	B	C
ATOM	1902	CG	TRP	B	557	32.130	28.109	78.514	1.00	2.60	B	C
ATOM	1903	CD2	TRP	B	557	31.217	27.477	77.614	1.00	1.31	B	C
ATOM	1904	CE2	TRP	B	557	30.435	26.577	78.373	1.00	1.25	B	C
ATOM	1905	CE3	TRP	B	557	30.980	27.583	76.240	1.00	0.43	B	C
ATOM	1906	CD1	TRP	B	557	31.874	27.583	79.748	1.00	2.55	B	C

ATOM	1907	NE1	TRP	B	557	30.858	26.662	79.672	1.00	0.74	B	N
ATOM	1908	CZ2	TRP	B	557	29.431	25.785	77.800	1.00	0.62	B	C
ATOM	1909	CZ3	TRP	B	557	29.976	26.793	75.670	1.00	0.00	B	C
ATOM	1910	CH2	TRP	B	557	29.217	25.908	76.452	1.00	0.00	B	C
ATOM	1911	C	TRP	B	557	31.518	30.699	77.119	1.00	5.06	B	C
ATOM	1912	O	TRP	B	557	31.673	30.894	75.910	1.00	4.78	B	O
ATOM	1913	N	ARG	B	558	30.331	30.570	77.703	1.00	5.26	B	N
ATOM	1914	CA	ARG	B	558	29.095	30.652	76.951	1.00	4.81	B	C
ATOM	1915	CB	ARG	B	558	27.922	30.183	77.822	1.00	5.22	B	C
ATOM	1916	CG	ARG	B	558	26.563	30.206	77.123	1.00	6.16	B	C
ATOM	1917	CD	ARG	B	558	25.538	29.316	77.807	1.00	9.34	B	C
ATOM	1918	NE	ARG	B	558	25.668	27.923	77.391	1.00	14.42	B	N
ATOM	1919	CZ	ARG	B	558	26.611	27.089	77.824	1.00	16.80	B	C
ATOM	1920	NH1	ARG	B	558	27.518	27.499	78.698	1.00	18.82	B	N
ATOM	1921	NH2	ARG	B	558	26.648	25.838	77.388	1.00	18.27	B	N
ATOM	1922	C	ARG	B	558	28.906	32.102	76.501	1.00	4.38	B	C
ATOM	1923	O	ARG	B	558	28.494	32.371	75.370	1.00	3.53	B	O
ATOM	1924	N	ILE	B	559	29.225	33.042	77.383	1.00	3.91	B	N
ATOM	1925	CA	ILE	B	559	29.096	34.443	77.021	1.00	3.73	B	C
ATOM	1926	CB	ILE	B	559	29.361	35.355	78.246	1.00	2.17	B	C
ATOM	1927	CG2	ILE	B	559	30.753	35.162	78.771	1.00	2.42	B	C
ATOM	1928	CG1	ILE	B	559	29.096	36.801	77.863	1.00	2.54	B	C
ATOM	1929	CD1	ILE	B	559	27.658	37.053	77.419	1.00	2.87	B	C
ATOM	1930	C	ILE	B	559	30.059	34.739	75.855	1.00	3.83	B	C
ATOM	1931	O	ILE	B	559	29.631	34.860	74.704	1.00	5.20	B	O
ATOM	1932	N	MET	B	560	31.352	34.825	76.147	1.00	2.87	B	N
ATOM	1933	CA	MET	B	560	32.363	35.063	75.128	1.00	1.24	B	C
ATOM	1934	CB	MET	B	560	33.721	34.619	75.639	1.00	1.99	B	C
ATOM	1935	CG	MET	B	560	34.211	35.458	76.789	1.00	2.39	B	C
ATOM	1936	SD	MET	B	560	34.293	37.166	76.285	1.00	4.27	B	S
ATOM	1937	CE	MET	B	560	35.496	37.085	74.934	1.00	4.41	B	C
ATOM	1938	C	MET	B	560	32.037	34.311	73.852	1.00	1.16	B	C
ATOM	1939	O	MET	B	560	32.311	34.780	72.750	1.00	1.87	B	O
ATOM	1940	N	THR	B	561	31.450	33.134	74.006	1.00	1.13	B	N
ATOM	1941	CA	THR	B	561	31.076	32.325	72.853	1.00	0.95	B	C
ATOM	1942	CB	THR	B	561	30.733	30.877	73.302	1.00	0.00	B	C
ATOM	1943	OG1	THR	B	561	31.953	30.181	73.595	1.00	0.00	B	O
ATOM	1944	CG2	THR	B	561	29.941	30.130	72.225	1.00	0.00	B	C
ATOM	1945	C	THR	B	561	29.881	32.969	72.129	1.00	1.92	B	C
ATOM	1946	O	THR	B	561	29.908	33.214	70.910	1.00	0.00	B	O
ATOM	1947	N	THR	B	562	28.835	33.259	72.889	1.00	3.03	B	N
ATOM	1948	CA	THR	B	562	27.667	33.869	72.306	1.00	4.11	B	C
ATOM	1949	CB	THR	B	562	26.582	34.048	73.366	1.00	2.50	B	C
ATOM	1950	OG1	THR	B	562	26.275	32.775	73.942	1.00	2.96	B	O
ATOM	1951	CG2	THR	B	562	25.323	34.623	72.751	1.00	4.08	B	C
ATOM	1952	C	THR	B	562	28.091	35.209	71.706	1.00	4.28	B	C
ATOM	1953	O	THR	B	562	27.543	35.636	70.685	1.00	5.63	B	O
ATOM	1954	N	LEU	B	563	29.077	35.862	72.330	1.00	4.35	B	N
ATOM	1955	CA	LEU	B	563	29.585	37.137	71.824	1.00	3.48	B	C
ATOM	1956	CB	LEU	B	563	30.657	37.709	72.742	1.00	1.87	B	C
ATOM	1957	CG	LEU	B	563	30.241	38.345	74.069	1.00	0.08	B	C
ATOM	1958	CD1	LEU	B	563	31.482	38.988	74.691	1.00	0.00	B	C
ATOM	1959	CD2	LEU	B	563	29.132	39.381	73.871	1.00	0.00	B	C
ATOM	1960	C	LEU	B	563	30.175	36.945	70.431	1.00	4.04	B	C
ATOM	1961	O	LEU	B	563	29.638	37.452	69.446	1.00	3.79	B	O
ATOM	1962	N	ASN	B	564	31.284	36.220	70.349	1.00	3.92	B	N
ATOM	1963	CA	ASN	B	564	31.920	35.931	69.066	1.00	4.06	B	C
ATOM	1964	CB	ASN	B	564	32.913	34.778	69.274	1.00	3.11	B	C
ATOM	1965	CG	ASN	B	564	33.637	34.379	68.009	1.00	2.95	B	C
ATOM	1966	OD1	ASN	B	564	33.198	33.488	67.283	1.00	3.54	B	O
ATOM	1967	ND2	ASN	B	564	34.754	35.041	67.736	1.00	2.53	B	C
ATOM	1968	C	ASN	B	564	30.853	35.573	68.005	1.00	4.42	B	C
ATOM	1969	O	ASN	B	564	31.005	35.879	66.818	1.00	2.35	B	O
ATOM	1970	N	MET	B	565	29.776	34.926	68.454	1.00	5.95	B	N
ATOM	1971	CA	MET	B	565	28.662	34.537	67.587	1.00	6.46	B	C
ATOM	1972	CB	MET	B	565	27.599	33.788	68.395	1.00	7.44	B	C
ATOM	1973	CG	MET	B	565	28.050	32.457	68.958	1.00	7.19	B	C
ATOM	1974	SD	MET	B	565	27.532	31.026	67.969	1.00	7.29	B	S
ATOM	1975	CE	MET	B	565	26.603	30.084	69.245	1.00	5.15	B	C
ATOM	1976	C	MET	B	565	28.034	35.788	66.993	1.00	6.14	B	C
ATOM	1977	O	MET	B	565	27.854	35.898	65.784	1.00	8.29	B	O
ATOM	1978	N	LEU	B	566	27.682	36.732	67.861	1.00	5.06	B	N
ATOM	1979	CA	LEU	B	566	27.089	37.977	67.403	1.00	3.90	B	C
ATOM	1980	CB	LEU	B	566	26.602	38.832	68.592	1.00	4.31	B	C
ATOM	1981	CG	LEU	B	566	25.656	40.018	68.309	1.00	0.27	B	C
ATOM	1982	CD1	LEU	B	566	24.411	39.579	67.570	1.00	0.00	B	C
ATOM	1983	CD2	LEU	B	566	25.262	40.657	69.604	1.00	0.00	B	C
ATOM	1984	C	LEU	B	566	28.220	38.668	66.681	1.00	3.90	B	C
ATOM	1985	O	LEU	B	566	28.071	39.766	66.177	1.00	5.32	B	O
ATOM	1986	N	GLY	B	567	29.362	37.998	66.630	1.00	2.58	B	N
ATOM	1987	CA	GLY	B	567	30.519	38.564	65.975	1.00	1.89	B	C

ATOM	1988	C	GLY	B	567	30.265	39.031	64.564	1.00	1.02	B	C
ATOM	1989	O	GLY	B	567	29.661	40.063	64.345	1.00	0.00	B	O
ATOM	1990	N	GLY	B	568	30.740	38.260	63.602	1.00	1.65	B	N
ATOM	1991	CA	GLY	B	568	30.573	38.623	62.213	1.00	2.01	B	C
ATOM	1992	C	GLY	B	568	29.151	38.957	61.832	1.00	2.92	B	C
ATOM	1993	O	GLY	B	568	28.912	39.563	60.785	1.00	4.64	B	O
ATOM	1994	N	ARG	B	569	28.199	38.561	62.667	1.00	3.12	B	N
ATOM	1995	CA	ARG	B	569	26.799	38.840	62.364	1.00	4.28	B	C
ATOM	1996	CB	ARG	B	569	25.874	38.031	63.292	1.00	4.60	B	C
ATOM	1997	CG	ARG	B	569	24.388	38.008	62.879	1.00	6.54	B	C
ATOM	1998	CD	ARG	B	569	23.552	37.402	63.995	1.00	6.72	B	C
ATOM	1999	NE	ARG	B	569	22.114	37.561	63.805	1.00	4.80	B	N
ATOM	2000	CZ	ARG	B	569	21.226	37.388	64.780	1.00	5.50	B	C
ATOM	2001	NH1	ARG	B	569	21.637	37.050	65.993	1.00	5.06	B	N
ATOM	2002	NH2	ARG	B	569	19.933	37.568	64.555	1.00	4.89	B	N
ATOM	2003	C	ARG	B	569	26.570	40.347	62.525	1.00	3.95	B	C
ATOM	2004	O	ARG	B	569	25.633	40.915	61.973	1.00	1.68	B	O
ATOM	2005	N	GLN	B	570	27.440	40.980	63.299	1.00	3.79	B	N
ATOM	2006	CA	GLN	B	570	27.368	42.402	63.506	1.00	2.90	B	C
ATOM	2007	CB	GLN	B	570	27.901	42.768	64.880	1.00	2.56	B	C
ATOM	2008	CG	GLN	B	570	27.054	42.267	66.003	1.00	4.22	B	C
ATOM	2009	CD	GLN	B	570	27.475	42.822	67.343	1.00	4.22	B	C
ATOM	2010	OE1	GLN	B	570	27.542	44.036	67.527	1.00	4.93	B	C
ATOM	2011	NE2	GLN	B	570	27.760	41.936	68.291	1.00	4.56	B	N
ATOM	2012	C	GLN	B	570	28.250	43.000	62.429	1.00	2.97	B	C
ATOM	2013	O	GLN	B	570	28.100	44.163	62.063	1.00	3.80	B	O
ATOM	2014	N	VAL	B	571	29.168	42.186	61.919	1.00	3.92	B	N
ATOM	2015	CA	VAL	B	571	30.093	42.612	60.868	1.00	4.74	B	C
ATOM	2016	CB	VAL	B	571	31.305	41.643	60.740	1.00	5.05	B	C
ATOM	2017	CG1	VAL	B	571	32.082	41.954	59.489	1.00	5.55	B	C
ATOM	2018	CG2	VAL	B	571	32.223	41.775	61.943	1.00	5.45	B	C
ATOM	2019	C	VAL	B	571	29.338	42.622	59.551	1.00	4.96	B	C
ATOM	2020	O	VAL	B	571	29.234	43.640	58.867	1.00	4.85	B	O
ATOM	2021	N	ILE	B	572	28.809	41.466	59.201	1.00	3.73	B	N
ATOM	2022	CA	ILE	B	572	28.049	41.331	57.986	1.00	2.14	B	C
ATOM	2023	CB	ILE	B	572	27.394	39.944	57.962	1.00	0.81	B	C
ATOM	2024	CG2	ILE	B	572	28.461	38.877	57.880	1.00	0.06	B	C
ATOM	2025	CG1	ILE	B	572	26.635	39.712	59.260	1.00	0.42	B	C
ATOM	2026	CD1	ILE	B	572	26.086	38.306	59.405	1.00	0.78	B	C
ATOM	2027	C	ILE	B	572	27.002	42.458	57.906	1.00	1.72	B	C
ATOM	2028	O	ILE	B	572	26.860	43.096	56.863	1.00	2.78	B	O
ATOM	2029	N	ALA	B	573	26.296	42.712	59.010	1.00	0.54	B	N
ATOM	2030	CA	ALA	B	573	25.275	43.762	59.058	1.00	0.88	B	C
ATOM	2031	CB	ALA	B	573	24.590	43.777	60.394	1.00	2.06	B	C
ATOM	2032	C	ALA	B	573	25.921	45.093	58.830	1.00	2.33	B	C
ATOM	2033	O	ALA	B	573	25.596	45.793	57.876	1.00	3.65	B	O
ATOM	2034	N	ALA	B	574	26.829	45.442	59.734	1.00	3.89	B	N
ATOM	2035	CA	ALA	B	574	27.568	46.693	59.646	1.00	4.51	B	C
ATOM	2036	CB	ALA	B	574	28.787	46.636	60.550	1.00	3.04	B	C
ATOM	2037	C	ALA	B	574	27.992	46.943	58.196	1.00	4.41	B	C
ATOM	2038	O	ALA	B	574	27.498	47.863	57.550	1.00	3.54	B	O
ATOM	2039	N	VAL	B	575	28.889	46.108	57.684	1.00	3.88	B	N
ATOM	2040	CA	VAL	B	575	29.371	46.246	56.313	1.00	4.05	B	C
ATOM	2041	CB	VAL	B	575	30.049	44.961	55.827	1.00	2.26	B	C
ATOM	2042	CG1	VAL	B	575	30.640	45.176	54.455	1.00	0.00	B	C
ATOM	2043	CG2	VAL	B	575	31.121	44.557	56.800	1.00	1.35	B	C
ATOM	2044	C	VAL	B	575	28.315	46.620	55.272	1.00	5.72	B	C
ATOM	2045	O	VAL	B	575	28.495	47.583	54.529	1.00	6.30	B	O
ATOM	2046	N	LYS	B	576	27.220	45.867	55.204	1.00	6.83	B	N
ATOM	2047	CA	LYS	B	576	26.176	46.148	54.215	1.00	6.98	B	C
ATOM	2048	CB	LYS	B	576	25.070	45.089	54.253	1.00	8.29	B	C
ATOM	2049	CG	LYS	B	576	24.060	45.198	53.102	1.00	9.99	B	C
ATOM	2050	CD	LYS	B	576	22.645	44.774	53.534	1.00	10.63	B	C
ATOM	2051	CE	LYS	B	576	21.998	45.820	54.458	1.00	10.34	B	C
ATOM	2052	NZ	LYS	B	576	21.917	47.184	53.831	1.00	9.62	B	N
ATOM	2053	C	LYS	B	576	25.565	47.507	54.480	1.00	5.53	B	C
ATOM	2054	O	LYS	B	576	24.880	48.071	53.619	1.00	7.34	B	O
ATOM	2055	N	TRP	B	577	25.786	48.011	55.689	1.00	3.30	B	N
ATOM	2056	CA	TRP	B	577	25.288	49.324	56.065	1.00	1.78	B	C
ATOM	2057	CB	TRP	B	577	25.156	49.425	57.575	1.00	0.84	B	C
ATOM	2058	CG	TRP	B	577	25.259	50.819	58.093	1.00	1.72	B	C
ATOM	2059	CD2	TRP	B	577	26.432	51.432	58.619	1.00	1.26	B	C
ATOM	2060	CE2	TRP	B	577	26.080	52.739	59.016	1.00	0.15	B	C
ATOM	2061	CE3	TRP	B	577	27.752	51.000	58.798	1.00	1.30	B	C
ATOM	2062	CD1	TRP	B	577	24.262	51.756	58.180	1.00	0.20	B	C
ATOM	2063	NE1	TRP	B	577	24.748	52.912	58.736	1.00	0.00	B	N
ATOM	2064	CZ2	TRP	B	577	27.004	53.618	59.583	1.00	2.91	B	C
ATOM	2065	CZ3	TRP	B	577	28.666	51.869	59.360	1.00	2.06	B	C
ATOM	2066	CH2	TRP	B	577	28.287	53.167	59.749	1.00	2.90	B	C
ATOM	2067	C	TRP	B	577	26.332	50.304	55.578	1.00	1.10	B	C
ATOM	2068	O	TRP	B	577	26.013	51.340	55.010	1.00	1.07	B	O

ATOM	2069	N	ALA	B	578	27.589	49.936	55.800	1.00	2.03	B	N
ATOM	2070	CA	ALA	B	578	28.736	50.737	55.402	1.00	2.60	B	C
ATOM	2071	CB	ALA	B	578	30.005	50.009	55.778	1.00	1.59	B	C
ATOM	2072	C	ALA	B	578	28.742	51.072	53.906	1.00	3.77	B	C
ATOM	2073	O	ALA	B	578	29.472	51.965	53.476	1.00	1.91	B	O
ATOM	2074	N	LYS	B	579	27.922	50.366	53.124	1.00	5.03	B	N
ATOM	2075	CA	LYS	B	579	27.834	50.593	51.675	1.00	5.31	B	C
ATOM	2076	CB	LYS	B	579	27.680	49.262	50.936	1.00	3.86	B	C
ATOM	2077	CG	LYS	B	579	28.997	48.566	50.650	1.00	5.98	B	C
ATOM	2078	CD	LYS	B	579	28.788	47.148	50.146	1.00	7.52	B	C
ATOM	2079	CE	LYS	B	579	28.199	46.251	51.239	1.00	8.30	B	C
ATOM	2080	NZ	LYS	B	579	29.106	46.143	52.421	1.00	8.68	B	N
ATOM	2081	C	LYS	B	579	26.707	51.534	51.255	1.00	4.99	B	C
ATOM	2082	O	LYS	B	579	26.700	52.049	50.135	1.00	5.31	B	O
ATOM	2083	N	ALA	B	580	25.756	51.758	52.152	1.00	4.36	B	N
ATOM	2084	CA	ALA	B	580	24.643	52.638	51.862	1.00	4.35	B	C
ATOM	2085	CB	ALA	B	580	23.398	52.083	52.483	1.00	5.65	B	C
ATOM	2086	C	ALA	B	580	24.923	54.052	52.382	1.00	4.33	B	C
ATOM	2087	O	ALA	B	580	24.046	54.914	52.374	1.00	5.33	B	O
ATOM	2088	N	ILE	B	581	26.149	54.278	52.851	1.00	3.84	B	N
ATOM	2089	CA	ILE	B	581	26.572	55.585	53.341	1.00	3.04	B	C
ATOM	2090	CB	ILE	B	581	27.966	55.530	53.999	1.00	0.00	B	C
ATOM	2091	CG2	ILE	B	581	28.272	56.839	54.669	1.00	0.00	B	C
ATOM	2092	CG1	ILE	B	581	28.043	54.385	55.006	1.00	0.00	B	C
ATOM	2093	CD1	ILE	B	581	26.965	54.404	56.055	1.00	0.00	B	C
ATOM	2094	C	ILE	B	581	26.705	56.403	52.070	1.00	3.79	B	C
ATOM	2095	O	ILE	B	581	27.506	56.070	51.202	1.00	3.83	B	O
ATOM	2096	N	PRO	B	582	25.904	57.463	51.923	1.00	3.55	B	N
ATOM	2097	CD	PRO	B	582	24.840	57.943	52.818	1.00	3.41	B	C
ATOM	2098	CA	PRO	B	582	25.975	58.298	50.728	1.00	3.83	B	C
ATOM	2099	CB	PRO	B	582	25.379	59.606	51.212	1.00	3.68	B	C
ATOM	2100	CG	PRO	B	582	24.229	59.105	52.024	1.00	3.46	B	C
ATOM	2101	C	PRO	B	582	27.380	58.444	50.166	1.00	3.53	B	C
ATOM	2102	O	PRO	B	582	28.297	58.926	50.835	1.00	1.92	B	O
ATOM	2103	N	GLY	B	583	27.539	57.999	48.928	1.00	3.25	B	N
ATOM	2104	CA	GLY	B	583	28.828	58.084	48.276	1.00	4.67	B	C
ATOM	2105	C	GLY	B	583	29.856	57.058	48.713	1.00	5.57	B	C
ATOM	2106	O	GLY	B	583	31.038	57.240	48.434	1.00	5.53	B	O
ATOM	2107	N	PHE	B	584	29.443	55.987	49.389	1.00	6.66	B	N
ATOM	2108	CA	PHE	B	584	30.424	54.992	49.795	1.00	8.01	B	C
ATOM	2109	CB	PHE	B	584	29.883	54.043	50.871	1.00	7.58	B	C
ATOM	2110	CG	PHE	B	584	30.975	53.337	51.657	1.00	7.47	B	C
ATOM	2111	CD1	PHE	B	584	31.735	54.032	52.610	1.00	7.09	B	C
ATOM	2112	CD2	PHE	B	584	31.281	51.997	51.409	1.00	6.32	B	C
ATOM	2113	CE1	PHE	B	584	32.788	53.398	53.301	1.00	6.01	B	C
ATOM	2114	CE2	PHE	B	584	32.327	51.362	52.093	1.00	6.56	B	C
ATOM	2115	CZ	PHE	B	584	33.082	52.063	53.038	1.00	6.03	B	C
ATOM	2116	C	PHE	B	584	30.846	54.189	48.575	1.00	8.32	B	C
ATOM	2117	O	PHE	B	584	32.039	53.992	48.353	1.00	9.53	B	O
ATOM	2118	N	ARG	B	585	29.883	53.723	47.784	1.00	8.64	B	N
ATOM	2119	CA	ARG	B	585	30.221	52.968	46.580	1.00	9.15	B	C
ATOM	2120	CB	ARG	B	585	28.990	52.696	45.723	1.00	11.66	B	C
ATOM	2121	CG	ARG	B	585	29.340	52.289	44.286	1.00	12.57	B	C
ATOM	2122	CD	ARG	B	585	28.101	52.081	43.440	1.00	13.14	B	C
ATOM	2123	NE	ARG	B	585	28.427	51.574	42.110	1.00	11.64	B	N
ATOM	2124	CZ	ARG	B	585	27.545	51.003	41.297	1.00	11.86	B	C
ATOM	2125	NH1	ARG	B	585	26.278	50.868	41.682	1.00	11.85	B	N
ATOM	2126	NH2	ARG	B	585	27.928	50.548	40.110	1.00	10.85	B	N
ATOM	2127	C	ARG	B	585	31.171	53.815	45.766	1.00	8.56	B	C
ATOM	2128	O	ARG	B	585	32.071	53.305	45.105	1.00	9.94	B	O
ATOM	2129	N	ASN	B	586	30.931	55.119	45.811	1.00	7.85	B	N
ATOM	2130	CA	ASN	B	586	31.732	56.109	45.112	1.00	7.35	B	C
ATOM	2131	CB	ASN	B	586	31.336	57.518	45.595	1.00	7.83	B	C
ATOM	2132	CG	ASN	B	586	29.975	57.985	45.043	1.00	7.05	B	C
ATOM	2133	OD1	ASN	B	586	29.909	58.958	44.273	1.00	6.99	B	O
ATOM	2134	ND2	ASN	B	586	28.891	57.300	45.438	1.00	7.50	B	N
ATOM	2135	C	ASN	B	586	33.233	55.870	45.343	1.00	6.72	B	C
ATOM	2136	O	ASN	B	586	34.055	56.071	44.444	1.00	5.85	B	O
ATOM	2137	N	LEU	B	587	33.585	55.433	46.549	1.00	5.45	B	N
ATOM	2138	CA	LEU	B	587	34.979	55.171	46.882	1.00	3.96	B	C
ATOM	2139	CB	LEU	B	587	35.186	55.130	48.401	1.00	2.16	B	C
ATOM	2140	CG	LEU	B	587	35.207	56.439	49.192	1.00	0.01	B	C
ATOM	2141	CD1	LEU	B	587	35.482	56.164	50.662	1.00	0.00	B	C
ATOM	2142	CD2	LEU	B	587	36.265	57.346	48.631	1.00	0.00	B	C
ATOM	2143	C	LEU	B	587	35.488	53.872	46.291	1.00	4.30	B	C
ATOM	2144	O	LEU	B	587	34.853	52.833	46.425	1.00	3.35	B	O
ATOM	2145	N	HIS	B	588	36.642	53.965	45.638	1.00	5.54	B	N
ATOM	2146	CA	HIS	B	588	37.341	52.838	45.017	1.00	6.10	B	C
ATOM	2147	CB	HIS	B	588	38.821	53.213	44.878	1.00	8.02	B	C
ATOM	2148	CG	HIS	B	588	39.615	52.300	43.998	1.00	9.78	B	C
ATOM	2149	CD2	HIS	B	588	39.287	51.141	43.380	1.00	10.15	B	C

ATOM	2150	ND1	HIS	B	588	40.922	52.566	43.647	1.00	9.69	B	N
ATOM	2151	CE1	HIS	B	588	41.364	51.613	42.849	1.00	10.29	B	C
ATOM	2152	NE2	HIS	B	588	40.392	50.736	42.670	1.00	10.23	B	N
ATOM	2153	C	HIS	B	588	37.190	51.655	45.962	1.00	5.17	B	C
ATOM	2154	O	HIS	B	588	37.183	51.847	47.178	1.00	6.61	B	O
ATOM	2155	N	LEU	B	589	37.062	50.439	45.439	1.00	3.01	B	N
ATOM	2156	CA	LEU	B	589	36.893	49.301	46.339	1.00	2.25	B	C
ATOM	2157	CB	LEU	B	589	36.698	48.001	45.560	1.00	2.93	B	C
ATOM	2158	CG	LEU	B	589	35.367	47.268	45.757	1.00	2.42	B	C
ATOM	2159	CD1	LEU	B	589	34.424	47.589	44.614	1.00	1.75	B	C
ATOM	2160	CD2	LEU	B	589	35.618	45.767	45.817	1.00	1.74	B	C
ATOM	2161	C	LEU	B	589	38.098	49.172	47.259	1.00	2.13	B	C
ATOM	2162	O	LEU	B	589	37.956	48.871	48.443	1.00	1.52	B	O
ATOM	2163	N	ASP	B	590	39.288	49.414	46.718	1.00	3.00	B	N
ATOM	2164	CA	ASP	B	590	40.503	49.318	47.518	1.00	4.35	B	C
ATOM	2165	CB	ASP	B	590	41.742	49.728	46.709	1.00	5.36	B	C
ATOM	2166	CG	ASP	B	590	42.349	48.573	45.915	1.00	6.32	B	C
ATOM	2167	OD1	ASP	B	590	41.753	48.150	44.901	1.00	6.81	B	O
ATOM	2168	OD2	ASP	B	590	43.433	48.087	46.311	1.00	7.64	B	O
ATOM	2169	C	ASP	B	590	40.355	50.237	48.712	1.00	4.59	B	C
ATOM	2170	O	ASP	B	590	41.149	50.181	49.645	1.00	4.53	B	O
ATOM	2171	N	ASP	B	591	39.338	51.094	48.655	1.00	5.18	B	N
ATOM	2172	CA	ASP	B	591	39.029	52.042	49.718	1.00	5.21	B	C
ATOM	2173	CB	ASP	B	591	38.178	53.183	49.182	1.00	6.04	B	C
ATOM	2174	CG	ASP	B	591	38.957	54.448	48.962	1.00	9.01	B	C
ATOM	2175	OD1	ASP	B	591	39.860	54.458	48.095	1.00	9.57	B	O
ATOM	2176	OD2	ASP	B	591	38.649	55.442	49.661	1.00	9.13	B	O
ATOM	2177	C	ASP	B	591	38.208	51.329	50.763	1.00	4.32	B	C
ATOM	2178	O	ASP	B	591	38.697	50.938	51.820	1.00	4.98	B	O
ATOM	2179	N	GLN	B	592	36.937	51.183	50.426	1.00	3.05	B	N
ATOM	2180	CA	GLN	B	592	35.930	50.544	51.255	1.00	2.86	B	C
ATOM	2181	CB	GLN	B	592	34.811	50.063	50.338	1.00	3.08	B	C
ATOM	2182	CG	GLN	B	592	34.422	51.132	49.332	1.00	2.00	B	C
ATOM	2183	CD	GLN	B	592	33.203	50.777	48.532	1.00	1.04	B	O
ATOM	2184	OE1	GLN	B	592	32.176	50.385	49.084	1.00	0.67	B	N
ATOM	2185	NE2	GLN	B	592	33.300	50.927	47.222	1.00	0.60	B	C
ATOM	2186	C	GLN	B	592	36.408	49.404	52.162	1.00	2.87	B	O
ATOM	2187	O	GLN	B	592	36.138	49.403	53.365	1.00	3.17	B	N
ATOM	2188	N	MET	B	593	37.102	48.427	51.595	1.00	2.27	B	C
ATOM	2189	CA	MET	B	593	37.582	47.330	52.406	1.00	0.85	B	C
ATOM	2190	CB	MET	B	593	38.289	46.290	51.546	1.00	0.46	B	C
ATOM	2191	CG	MET	B	593	37.516	45.838	50.328	1.00	0.00	B	S
ATOM	2192	SD	MET	B	593	36.312	44.532	50.608	1.00	0.00	B	C
ATOM	2193	CE	MET	B	593	36.060	43.971	48.905	1.00	0.00	B	C
ATOM	2194	C	MET	B	593	38.569	47.917	53.398	1.00	0.54	B	O
ATOM	2195	O	MET	B	593	38.626	47.499	54.548	1.00	0.38	B	N
ATOM	2196	N	THR	B	594	39.339	48.905	52.960	1.00	0.01	B	C
ATOM	2197	CA	THR	B	594	40.329	49.504	53.837	1.00	0.90	B	C
ATOM	2198	CB	THR	B	594	41.279	50.423	53.074	1.00	2.47	B	O
ATOM	2199	OG1	THR	B	594	41.818	49.727	51.948	1.00	5.59	B	C
ATOM	2200	CG2	THR	B	594	42.435	50.820	53.967	1.00	5.05	B	C
ATOM	2201	C	THR	B	594	39.747	50.293	54.992	1.00	0.05	B	O
ATOM	2202	O	THR	B	594	40.286	50.267	56.091	1.00	0.00	B	N
ATOM	2203	N	LEU	B	595	38.651	50.998	54.751	1.00	0.00	B	C
ATOM	2204	CA	LEU	B	595	38.038	51.794	55.803	1.00	0.00	B	C
ATOM	2205	CB	LEU	B	595	37.328	52.999	55.216	1.00	0.00	B	C
ATOM	2206	CG	LEU	B	595	38.258	53.979	54.518	1.00	0.00	B	C
ATOM	2207	CD1	LEU	B	595	37.435	55.089	53.859	1.00	0.00	B	C
ATOM	2208	CD2	LEU	B	595	39.259	54.525	55.532	1.00	0.00	B	C
ATOM	2209	C	LEU	B	595	37.061	50.988	56.612	1.00	0.00	B	O
ATOM	2210	O	LEU	B	595	36.399	51.522	57.496	1.00	0.00	B	N
ATOM	2211	N	LEU	B	596	36.964	49.700	56.296	1.00	0.00	B	C
ATOM	2212	CA	LEU	B	596	36.077	48.795	57.021	1.00	0.00	B	C
ATOM	2213	CB	LEU	B	596	35.292	47.912	56.056	1.00	0.00	B	C
ATOM	2214	CG	LEU	B	596	33.949	48.554	55.731	1.00	0.00	B	C
ATOM	2215	CD1	LEU	B	596	33.474	48.116	54.388	1.00	0.00	B	C
ATOM	2216	CD2	LEU	B	596	32.963	48.196	56.804	1.00	0.00	B	C
ATOM	2217	C	LEU	B	596	36.851	47.943	58.011	1.00	0.00	B	O
ATOM	2218	O	LEU	B	596	36.283	47.424	58.956	1.00	0.00	B	N
ATOM	2219	N	GLN	B	597	38.154	47.819	57.807	1.00	0.00	B	C
ATOM	2220	CA	GLN	B	597	38.976	47.046	58.721	1.00	0.00	B	C
ATOM	2221	CB	GLN	B	597	40.198	46.492	57.996	1.00	0.00	B	C
ATOM	2222	CG	GLN	B	597	39.923	46.078	56.563	1.00	0.00	B	C
ATOM	2223	CD	GLN	B	597	41.148	45.542	55.855	1.00	0.00	B	O
ATOM	2224	OE1	GLN	B	597	41.175	45.458	54.632	1.00	0.27	B	N
ATOM	2225	NE2	GLN	B	597	42.169	45.171	56.621	1.00	0.83	B	C
ATOM	2226	C	GLN	B	597	39.426	47.982	59.827	1.00	0.84	B	O
ATOM	2227	O	GLN	B	597	40.029	47.551	60.804	1.00	0.26	B	N
ATOM	2228	N	TYR	B	598	39.120	49.270	59.657	1.00	2.28	B	C
ATOM	2229	CA	TYR	B	598	39.497	50.311	60.615	1.00	1.69	B	C
ATOM	2230	CB	TYR	B	598	40.023	51.568	59.904	1.00	0.89	B	C

ATOM	2231	CG	TYR	B	598	41.431	51.442	59.379	1.00	0.31	B	C
ATOM	2232	CD1	TYR	B	598	42.385	50.740	60.097	1.00	1.10	B	C
ATOM	2233	CE1	TYR	B	598	43.677	50.588	59.616	1.00	2.81	B	C
ATOM	2234	CD2	TYR	B	598	41.804	52.004	58.156	1.00	0.59	B	C
ATOM	2235	CE2	TYR	B	598	43.105	51.859	57.662	1.00	1.23	B	C
ATOM	2236	CZ	TYR	B	598	44.035	51.145	58.405	1.00	1.88	B	C
ATOM	2237	OH	TYR	B	598	45.327	50.968	57.973	1.00	2.15	B	O
ATOM	2238	C	TYR	B	598	38.377	50.747	61.515	1.00	1.61	B	C
ATOM	2239	O	TYR	B	598	38.623	51.163	62.635	1.00	1.98	B	O
ATOM	2240	N	SER	B	599	37.146	50.674	61.033	1.00	1.16	B	N
ATOM	2241	CA	SER	B	599	36.035	51.116	61.856	1.00	2.83	B	C
ATOM	2242	CB	SER	B	599	35.127	52.092	61.084	1.00	4.32	B	C
ATOM	2243	OG	SER	B	599	34.697	51.588	59.833	1.00	3.44	B	O
ATOM	2244	C	SER	B	599	35.196	50.023	62.451	1.00	4.52	B	C
ATOM	2245	O	SER	B	599	34.324	50.300	63.268	1.00	4.40	B	O
ATOM	2246	N	TRP	B	600	35.443	48.780	62.073	1.00	6.24	B	N
ATOM	2247	CA	TRP	B	600	34.613	47.743	62.635	1.00	6.32	B	C
ATOM	2248	CB	TRP	B	600	35.102	46.339	62.240	1.00	7.27	B	C
ATOM	2249	CG	TRP	B	600	36.458	45.987	62.660	1.00	5.88	B	C
ATOM	2250	CD2	TRP	B	600	36.811	44.996	63.619	1.00	7.07	B	C
ATOM	2251	CE2	TRP	B	600	38.217	44.960	63.683	1.00	7.93	B	C
ATOM	2252	CE3	TRP	B	600	36.075	44.128	64.430	1.00	8.44	B	C
ATOM	2253	CD1	TRP	B	600	37.621	46.507	62.193	1.00	6.78	B	C
ATOM	2254	NE1	TRP	B	600	38.690	45.895	62.801	1.00	7.75	B	N
ATOM	2255	CZ2	TRP	B	600	38.905	44.087	64.534	1.00	7.05	B	C
ATOM	2256	CZ3	TRP	B	600	36.761	43.257	65.276	1.00	8.68	B	C
ATOM	2257	CH2	TRP	B	600	38.160	43.246	65.319	1.00	7.49	B	C
ATOM	2258	C	TRP	B	600	34.542	47.925	64.146	1.00	5.61	B	C
ATOM	2259	O	TRP	B	600	33.509	48.348	64.666	1.00	5.39	B	O
ATOM	2260	N	MET	B	601	35.627	47.657	64.858	1.00	2.99	B	N
ATOM	2261	CA	MET	B	601	35.587	47.824	66.304	1.00	1.29	B	C
ATOM	2262	CB	MET	B	601	36.930	47.461	66.925	1.00	1.89	B	C
ATOM	2263	CG	MET	B	601	36.902	46.210	67.778	1.00	0.00	B	C
ATOM	2264	SD	MET	B	601	36.169	46.459	69.382	1.00	0.00	B	S
ATOM	2265	CE	MET	B	601	34.471	46.044	69.045	1.00	0.00	B	C
ATOM	2266	C	MET	B	601	35.186	49.236	66.726	1.00	1.02	B	C
ATOM	2267	O	MET	B	601	35.027	49.503	67.909	1.00	1.15	B	O
ATOM	2268	N	PHE	B	602	35.035	50.147	65.775	1.00	1.01	B	N
ATOM	2269	CA	PHE	B	602	34.605	51.495	66.127	1.00	1.34	B	C
ATOM	2270	CB	PHE	B	602	35.014	52.503	65.052	1.00	2.99	B	C
ATOM	2271	CG	PHE	B	602	36.464	52.867	65.090	1.00	2.66	B	C
ATOM	2272	CD1	PHE	B	602	37.074	53.438	63.983	1.00	3.07	B	C
ATOM	2273	CD2	PHE	B	602	37.222	52.627	66.228	1.00	2.91	B	C
ATOM	2274	CE1	PHE	B	602	38.419	53.758	64.003	1.00	4.19	B	C
ATOM	2275	CE2	PHE	B	602	38.568	52.941	66.266	1.00	4.37	B	C
ATOM	2276	CZ	PHE	B	602	39.174	53.507	65.151	1.00	4.32	B	C
ATOM	2277	C	PHE	B	602	33.101	51.419	66.207	1.00	1.47	B	C
ATOM	2278	O	PHE	B	602	32.501	51.768	67.218	1.00	0.00	B	O
ATOM	2279	N	LEU	B	603	32.514	50.935	65.117	1.00	1.98	B	N
ATOM	2280	CA	LEU	B	603	31.074	50.748	64.993	1.00	2.50	B	C
ATOM	2281	CB	LEU	B	603	30.758	50.146	63.622	1.00	2.06	B	C
ATOM	2282	CG	LEU	B	603	31.368	50.917	62.449	1.00	2.73	B	C
ATOM	2283	CD1	LEU	B	603	31.333	50.088	61.172	1.00	1.78	B	C
ATOM	2284	CD2	LEU	B	603	30.617	52.228	62.279	1.00	3.65	B	C
ATOM	2285	C	LEU	B	603	30.594	49.802	66.105	1.00	2.05	B	C
ATOM	2286	O	LEU	B	603	29.738	50.159	66.921	1.00	3.14	B	O
ATOM	2287	N	MET	B	604	31.163	48.597	66.128	1.00	0.08	B	N
ATOM	2288	CA	MET	B	604	30.836	47.586	67.127	1.00	0.00	B	C
ATOM	2289	CB	MET	B	604	31.908	46.508	67.117	1.00	0.00	B	C
ATOM	2290	CG	MET	B	604	32.152	45.881	65.760	1.00	0.00	B	C
ATOM	2291	SD	MET	B	604	30.756	44.948	65.192	1.00	0.00	B	S
ATOM	2292	CE	MET	B	604	30.508	43.905	66.564	1.00	0.00	B	C
ATOM	2293	C	MET	B	604	30.769	48.193	68.520	1.00	0.00	B	C
ATOM	2294	O	MET	B	604	29.738	48.145	69.187	1.00	0.00	B	O
ATOM	2295	N	ALA	B	605	31.896	48.756	68.943	1.00	0.00	B	N
ATOM	2296	CA	ALA	B	605	32.051	49.391	70.249	1.00	0.00	B	C
ATOM	2297	CB	ALA	B	605	33.512	49.755	70.484	1.00	0.00	B	C
ATOM	2298	C	ALA	B	605	31.204	50.633	70.389	1.00	0.00	B	C
ATOM	2299	O	ALA	B	605	30.745	50.970	71.474	1.00	0.00	B	O
ATOM	2300	N	PHE	B	606	31.007	51.342	69.297	1.00	0.00	B	N
ATOM	2301	CA	PHE	B	606	30.193	52.519	69.415	1.00	0.00	B	C
ATOM	2302	CB	PHE	B	606	30.303	53.388	68.171	1.00	0.00	B	C
ATOM	2303	CG	PHE	B	606	29.828	54.790	68.388	1.00	0.00	B	C
ATOM	2304	CD1	PHE	B	606	30.284	55.523	69.469	1.00	0.00	B	C
ATOM	2305	CD2	PHE	B	606	28.911	55.364	67.533	1.00	0.00	B	C
ATOM	2306	CE1	PHE	B	606	29.831	56.796	69.694	1.00	0.00	B	C
ATOM	2307	CE2	PHE	B	606	28.454	56.636	67.749	1.00	0.00	B	C
ATOM	2308	CZ	PHE	B	606	28.913	57.358	68.832	1.00	0.00	B	C
ATOM	2309	C	PHE	B	606	28.779	52.039	69.594	1.00	0.00	B	C
ATOM	2310	O	PHE	B	606	28.214	52.143	70.672	1.00	0.00	B	O
ATOM	2311	N	ALA	B	607	28.228	51.486	68.526	1.00	0.00	B	N

ATOM	2312	CA	ALA	B	607	26.873	50.968	68.521	1.00	0.00	B	C
ATOM	2313	CB	ALA	B	607	26.756	49.879	67.486	1.00	0.56	B	C
ATOM	2314	C	ALA	B	607	26.437	50.439	69.878	1.00	0.91	B	C
ATOM	2315	O	ALA	B	607	25.330	50.718	70.342	1.00	1.76	B	O
ATOM	2316	N	LEU	B	608	27.310	49.678	70.518	1.00	1.36	B	N
ATOM	2317	CA	LEU	B	608	26.989	49.111	71.814	1.00	2.10	B	C
ATOM	2318	CB	LEU	B	608	27.997	48.045	72.197	1.00	3.39	B	C
ATOM	2319	CG	LEU	B	608	27.644	47.457	73.560	1.00	3.27	B	C
ATOM	2320	CD1	LEU	B	608	26.337	46.695	73.435	1.00	3.39	B	C
ATOM	2321	CD2	LEU	B	608	28.762	46.568	74.053	1.00	3.51	B	C
ATOM	2322	C	LEU	B	608	26.937	50.126	72.937	1.00	1.59	B	C
ATOM	2323	O	LEU	B	608	26.060	50.045	73.796	1.00	2.42	B	O
ATOM	2324	N	GLY	B	609	27.900	51.048	72.954	1.00	0.59	B	N
ATOM	2325	CA	GLY	B	609	27.929	52.068	73.988	1.00	0.00	B	C
ATOM	2326	C	GLY	B	609	26.622	52.835	73.958	1.00	0.00	B	C
ATOM	2327	O	GLY	B	609	26.097	53.246	74.991	1.00	0.00	B	O
ATOM	2328	N	TRP	B	610	26.094	53.014	72.753	1.00	0.00	B	N
ATOM	2329	CA	TRP	B	610	24.837	53.710	72.552	1.00	0.00	B	C
ATOM	2330	CB	TRP	B	610	24.677	54.111	71.093	1.00	0.16	B	C
ATOM	2331	CG	TRP	B	610	23.343	54.693	70.802	1.00	0.72	B	C
ATOM	2332	CD2	TRP	B	610	23.011	56.080	70.798	1.00	1.34	B	C
ATOM	2333	CE2	TRP	B	610	21.623	56.177	70.568	1.00	2.02	B	C
ATOM	2334	CE3	TRP	B	610	23.754	57.254	70.975	1.00	0.48	B	C
ATOM	2335	CD1	TRP	B	610	22.180	54.016	70.574	1.00	1.46	B	C
ATOM	2336	NE1	TRP	B	610	21.139	54.903	70.433	1.00	2.17	B	N
ATOM	2337	CZ2	TRP	B	610	20.961	57.403	70.510	1.00	1.13	B	C
ATOM	2338	CZ3	TRP	B	610	23.098	58.469	70.918	1.00	0.00	B	C
ATOM	2339	CH2	TRP	B	610	21.714	58.536	70.688	1.00	0.11	B	C
ATOM	2340	C	TRP	B	610	23.695	52.799	72.927	1.00	0.00	B	C
ATOM	2341	O	TRP	B	610	22.831	53.156	73.725	1.00	0.00	B	O
ATOM	2342	N	ARG	B	611	23.681	51.621	72.321	1.00	0.00	B	N
ATOM	2343	CA	ARG	B	611	22.639	50.656	72.615	1.00	0.00	B	C
ATOM	2344	CB	ARG	B	611	22.950	49.306	71.964	1.00	0.00	B	C
ATOM	2345	CG	ARG	B	611	22.234	49.049	70.647	1.00	0.00	B	C
ATOM	2346	CD	ARG	B	611	22.456	47.626	70.171	1.00	0.00	B	C
ATOM	2347	NE	ARG	B	611	23.668	47.457	69.376	1.00	0.00	B	N
ATOM	2348	CZ	ARG	B	611	23.809	47.897	68.129	1.00	0.00	B	C
ATOM	2349	NH1	ARG	B	611	22.817	48.547	67.529	1.00	0.00	B	N
ATOM	2350	NH2	ARG	B	611	24.930	47.656	67.465	1.00	0.00	B	N
ATOM	2351	C	ARG	B	611	22.485	50.470	74.119	1.00	0.00	B	C
ATOM	2352	O	ARG	B	611	21.393	50.608	74.650	1.00	0.00	B	O
ATOM	2353	N	SER	B	612	23.586	50.176	74.799	1.00	0.21	B	N
ATOM	2354	CA	SER	B	612	23.559	49.949	76.240	1.00	1.64	B	C
ATOM	2355	CB	SER	B	612	24.752	49.108	76.671	1.00	1.97	B	C
ATOM	2356	OG	SER	B	612	25.962	49.774	76.377	1.00	3.40	B	O
ATOM	2357	C	SER	B	612	23.570	51.221	77.043	1.00	2.58	B	C
ATOM	2358	O	SER	B	612	24.271	51.309	78.042	1.00	1.68	B	O
ATOM	2359	N	TYR	B	613	22.794	52.201	76.599	1.00	3.97	B	N
ATOM	2360	CA	TYR	B	613	22.682	53.493	77.269	1.00	4.63	B	C
ATOM	2361	CB	TYR	B	613	23.712	54.484	76.691	1.00	5.30	B	C
ATOM	2362	CG	TYR	B	613	23.203	55.901	76.397	1.00	6.54	B	C
ATOM	2363	CD1	TYR	B	613	23.561	56.980	77.206	1.00	7.05	B	C
ATOM	2364	CE1	TYR	B	613	23.136	58.282	76.913	1.00	5.11	B	C
ATOM	2365	CD2	TYR	B	613	22.398	56.165	75.282	1.00	6.80	B	C
ATOM	2366	CE2	TYR	B	613	21.967	57.466	74.982	1.00	5.86	B	C
ATOM	2367	CZ	TYR	B	613	22.344	58.510	75.804	1.00	5.00	B	C
ATOM	2368	OH	TYR	B	613	21.931	59.782	75.517	1.00	4.53	B	O
ATOM	2369	C	TYR	B	613	21.276	53.996	77.040	1.00	4.58	B	C
ATOM	2370	O	TYR	B	613	20.830	54.931	77.689	1.00	5.04	B	O
ATOM	2371	N	ARG	B	614	20.588	53.349	76.109	1.00	5.02	B	N
ATOM	2372	CA	ARG	B	614	19.238	53.721	75.741	1.00	5.62	B	C
ATOM	2373	CB	ARG	B	614	19.226	53.987	74.227	1.00	5.50	B	C
ATOM	2374	CG	ARG	B	614	17.995	54.664	73.612	1.00	4.73	B	C
ATOM	2375	CD	ARG	B	614	18.203	54.848	72.099	1.00	3.65	B	C
ATOM	2376	NE	ARG	B	614	16.987	55.193	71.360	1.00	4.58	B	N
ATOM	2377	CZ	ARG	B	614	16.852	55.070	70.036	1.00	3.71	B	C
ATOM	2378	NH1	ARG	B	614	17.860	54.607	69.313	1.00	3.92	B	N
ATOM	2379	NH2	ARG	B	614	15.717	55.415	69.425	1.00	2.03	B	N
ATOM	2380	C	ARG	B	614	18.253	52.599	76.122	1.00	6.34	B	C
ATOM	2381	O	ARG	B	614	17.164	52.868	76.645	1.00	6.10	B	O
ATOM	2382	N	GLN	B	615	18.653	51.346	75.890	1.00	6.19	B	N
ATOM	2383	CA	GLN	B	615	17.798	50.183	76.148	1.00	5.85	B	C
ATOM	2384	CB	GLN	B	615	17.929	49.190	74.992	1.00	6.52	B	C
ATOM	2385	CG	GLN	B	615	17.105	49.543	73.762	1.00	10.40	B	C
ATOM	2386	CD	GLN	B	615	15.605	49.275	73.938	1.00	12.10	B	C
ATOM	2387	OE1	GLN	B	615	14.794	49.647	73.081	1.00	12.21	B	O
ATOM	2388	NE2	GLN	B	615	15.234	48.616	75.043	1.00	13.67	B	N
ATOM	2389	C	GLN	B	615	17.965	49.424	77.455	1.00	5.32	B	C
ATOM	2390	O	GLN	B	615	17.735	48.208	77.500	1.00	2.66	B	O
ATOM	2391	N	SER	B	616	18.359	50.127	78.514	1.00	5.88	B	N
ATOM	2392	CA	SER	B	616	18.525	49.491	79.826	1.00	6.22	B	C

ATOM	2393	CB	SER	B	616	19.477	48.281	79.729	1.00	4.53	B	C
ATOM	2394	OG	SER	B	616	19.024	47.204	80.538	1.00	4.21	B	O
ATOM	2395	C	SER	B	616	19.044	50.504	80.846	1.00	6.59	B	C
ATOM	2396	O	SER	B	616	19.244	50.172	82.017	1.00	6.15	B	O
ATOM	2397	N	SER	B	617	19.239	51.736	80.373	1.00	6.95	B	N
ATOM	2398	CA	SER	B	617	19.720	52.865	81.175	1.00	8.12	B	C
ATOM	2399	CB	SER	B	617	19.317	52.732	82.651	1.00	9.42	B	C
ATOM	2400	OG	SER	B	617	19.909	53.759	83.441	1.00	10.49	B	O
ATOM	2401	C	SER	B	617	21.221	53.050	81.104	1.00	8.93	B	C
ATOM	2402	O	SER	B	617	21.773	53.880	81.825	1.00	9.37	B	O
ATOM	2403	N	ALA	B	618	21.875	52.271	80.247	1.00	9.92	B	N
ATOM	2404	CA	ALA	B	618	23.322	52.345	80.065	1.00	10.07	B	C
ATOM	2405	CB	ALA	B	618	23.771	53.817	80.062	1.00	10.64	B	C
ATOM	2406	C	ALA	B	618	24.196	51.540	81.036	1.00	9.64	B	C
ATOM	2407	O	ALA	B	618	24.943	50.652	80.616	1.00	8.47	B	O
ATOM	2408	N	ASN	B	619	24.095	51.865	82.326	1.00	8.32	B	N
ATOM	2409	CA	ASN	B	619	24.879	51.235	83.405	1.00	6.30	B	C
ATOM	2410	CB	ASN	B	619	24.340	51.713	84.765	1.00	5.29	B	C
ATOM	2411	CG	ASN	B	619	25.405	51.720	85.836	1.00	6.28	B	C
ATOM	2412	OD1	ASN	B	619	26.542	52.116	85.585	1.00	6.67	B	O
ATOM	2413	ND2	ASN	B	619	25.043	51.292	87.042	1.00	6.41	B	N
ATOM	2414	C	ASN	B	619	24.959	49.692	83.368	1.00	4.39	B	C
ATOM	2415	O	ASN	B	619	25.668	49.070	84.169	1.00	1.39	B	O
ATOM	2416	N	LEU	B	620	24.220	49.104	82.430	1.00	3.21	B	N
ATOM	2417	CA	LEU	B	620	24.183	47.675	82.213	1.00	1.64	B	C
ATOM	2418	CB	LEU	B	620	22.770	47.146	82.396	1.00	0.00	B	C
ATOM	2419	CG	LEU	B	620	22.061	47.375	83.728	1.00	0.00	B	C
ATOM	2420	CD1	LEU	B	620	20.949	46.362	83.847	1.00	0.00	B	C
ATOM	2421	CD2	LEU	B	620	23.003	47.209	84.886	1.00	0.00	B	C
ATOM	2422	C	LEU	B	620	24.613	47.471	80.769	1.00	1.61	B	C
ATOM	2423	O	LEU	B	620	24.020	48.057	79.869	1.00	3.95	B	O
ATOM	2424	N	LEU	B	621	25.638	46.650	80.550	1.00	0.61	B	N
ATOM	2425	CA	LEU	B	621	26.161	46.380	79.209	1.00	0.00	B	C
ATOM	2426	CB	LEU	B	621	27.537	45.748	79.337	1.00	0.29	B	C
ATOM	2427	CG	LEU	B	621	28.725	46.661	79.086	1.00	0.00	B	C
ATOM	2428	CD1	LEU	B	621	30.006	45.916	79.397	1.00	0.00	B	C
ATOM	2429	CD2	LEU	B	621	28.719	47.123	77.636	1.00	0.00	B	C
ATOM	2430	C	LEU	B	621	25.282	45.498	78.309	1.00	0.00	B	C
ATOM	2431	O	LEU	B	621	25.510	44.303	78.199	1.00	0.00	B	O
ATOM	2432	N	CYS	B	622	24.309	46.096	77.633	1.00	0.00	B	N
ATOM	2433	CA	CYS	B	622	23.410	45.334	76.781	1.00	0.00	B	C
ATOM	2434	CB	CYS	B	622	22.015	45.958	76.803	1.00	0.00	B	C
ATOM	2435	SG	CYS	B	622	21.856	47.444	75.813	1.00	0.00	B	S
ATOM	2436	C	CYS	B	622	23.857	45.177	75.332	1.00	0.00	B	C
ATOM	2437	O	CYS	B	622	23.734	46.100	74.525	1.00	0.00	B	O
ATOM	2438	N	PHE	B	623	24.328	43.977	75.005	1.00	0.00	B	N
ATOM	2439	CA	PHE	B	623	24.797	43.638	73.668	1.00	0.00	B	C
ATOM	2440	CB	PHE	B	623	25.745	42.469	73.775	1.00	0.00	B	C
ATOM	2441	CG	PHE	B	623	26.936	42.756	74.616	1.00	0.00	B	C
ATOM	2442	CD1	PHE	B	623	28.108	43.213	74.046	1.00	0.00	B	C
ATOM	2443	CD2	PHE	B	623	26.891	42.561	75.982	1.00	0.00	B	C
ATOM	2444	CE1	PHE	B	623	29.225	43.467	74.828	1.00	0.00	B	C
ATOM	2445	CE2	PHE	B	623	28.003	42.814	76.775	1.00	0.00	B	C
ATOM	2446	CZ	PHE	B	623	29.171	43.266	76.195	1.00	0.00	B	C
ATOM	2447	C	PHE	B	623	23.686	43.311	72.683	1.00	0.40	B	C
ATOM	2448	O	PHE	B	623	23.933	43.140	71.496	1.00	0.00	B	O
ATOM	2449	N	ALA	B	624	22.464	43.233	73.195	1.00	2.69	B	N
ATOM	2450	CA	ALA	B	624	21.275	42.929	72.401	1.00	3.96	B	C
ATOM	2451	CB	ALA	B	624	21.515	41.705	71.532	1.00	4.93	B	C
ATOM	2452	C	ALA	B	624	20.114	42.664	73.352	1.00	5.05	B	C
ATOM	2453	O	ALA	B	624	20.255	42.806	74.559	1.00	6.07	B	O
ATOM	2454	N	PRO	B	625	18.943	42.289	72.820	1.00	6.15	B	N
ATOM	2455	CD	PRO	B	625	18.440	42.525	71.457	1.00	8.05	B	C
ATOM	2456	CA	PRO	B	625	17.826	42.028	73.729	1.00	6.77	B	C
ATOM	2457	CB	PRO	B	625	16.619	42.001	72.790	1.00	7.53	B	C
ATOM	2458	CG	PRO	B	625	17.007	42.951	71.718	1.00	7.37	B	C
ATOM	2459	C	PRO	B	625	17.979	40.720	74.510	1.00	7.14	B	C
ATOM	2460	O	PRO	B	625	17.798	40.693	75.734	1.00	8.70	B	O
ATOM	2461	N	ASP	B	626	18.306	39.642	73.798	1.00	6.33	B	N
ATOM	2462	CA	ASP	B	626	18.464	38.329	74.422	1.00	4.49	B	C
ATOM	2463	CB	ASP	B	626	18.615	37.233	73.350	1.00	3.52	B	C
ATOM	2464	CG	ASP	B	626	19.524	37.646	72.200	1.00	1.47	B	C
ATOM	2465	OD1	ASP	B	626	19.009	38.023	71.128	1.00	1.35	B	O
ATOM	2466	OD2	ASP	B	626	20.754	37.599	72.366	1.00	0.00	B	O
ATOM	2467	C	ASP	B	626	19.648	38.280	75.375	1.00	3.48	B	C
ATOM	2468	O	ASP	B	626	19.825	37.307	76.110	1.00	4.01	B	O
ATOM	2469	N	LEU	B	627	20.434	39.351	75.390	1.00	2.34	B	N
ATOM	2470	CA	LEU	B	627	21.617	39.387	76.231	1.00	1.42	B	C
ATOM	2471	CB	LEU	B	627	22.792	38.934	75.385	1.00	1.67	B	C
ATOM	2472	CG	LEU	B	627	24.138	38.855	76.059	1.00	3.87	B	C
ATOM	2473	CD1	LEU	B	627	23.967	38.520	77.535	1.00	5.30	B	C

ATOM	2474	CD2	LEU	B	627	24.961	37.791	75.328	1.00	5.56	B	C
ATOM	2475	C	LEU	B	627	21.915	40.750	76.859	1.00	0.98	B	C
ATOM	2476	O	LEU	B	627	22.050	41.739	76.160	1.00	0.00	B	O
ATOM	2477	N	ILE	B	628	22.015	40.804	78.181	1.00	1.05	B	N
ATOM	2478	CA	ILE	B	628	22.302	42.063	78.861	1.00	0.28	B	C
ATOM	2479	CB	ILE	B	628	21.020	42.771	79.358	1.00	0.00	B	C
ATOM	2480	CG2	ILE	B	628	21.298	44.242	79.573	1.00	0.00	B	C
ATOM	2481	CG1	ILE	B	628	19.893	42.621	78.346	1.00	0.33	B	C
ATOM	2482	CD1	ILE	B	628	19.159	41.291	78.449	1.00	1.09	B	C
ATOM	2483	C	ILE	B	628	23.188	41.820	80.077	1.00	0.23	B	C
ATOM	2484	O	ILE	B	628	22.703	41.640	81.195	1.00	0.00	B	O
ATOM	2485	N	ILE	B	629	24.493	41.821	79.875	1.00	0.02	B	N
ATOM	2486	CA	ILE	B	629	25.344	41.573	81.004	1.00	1.90	B	C
ATOM	2487	CB	ILE	B	629	26.817	41.730	80.660	1.00	0.66	B	C
ATOM	2488	CG2	ILE	B	629	27.666	41.522	81.917	1.00	0.00	B	C
ATOM	2489	CG1	ILE	B	629	27.189	40.703	79.595	1.00	0.31	B	C
ATOM	2490	CD1	ILE	B	629	28.646	40.608	79.345	1.00	0.44	B	C
ATOM	2491	C	ILE	B	629	24.995	42.498	82.139	1.00	3.45	B	C
ATOM	2492	O	ILE	B	629	25.280	43.680	82.083	1.00	4.49	B	O
ATOM	2493	N	ASN	B	630	24.359	41.943	83.163	1.00	4.89	B	N
ATOM	2494	CA	ASN	B	630	23.965	42.677	84.365	1.00	5.30	B	C
ATOM	2495	CB	ASN	B	630	23.366	41.681	85.352	1.00	3.90	B	C
ATOM	2496	CG	ASN	B	630	22.374	40.745	84.684	1.00	5.42	B	C
ATOM	2497	OD1	ASN	B	630	22.685	40.127	83.659	1.00	4.80	B	O
ATOM	2498	ND2	ASN	B	630	21.173	40.637	85.254	1.00	4.96	B	N
ATOM	2499	C	ASN	B	630	25.185	43.370	84.971	1.00	5.91	B	C
ATOM	2500	O	ASN	B	630	26.053	43.825	84.242	1.00	5.56	B	O
ATOM	2501	N	GLU	B	631	25.272	43.462	86.293	1.00	7.42	B	N
ATOM	2502	CA	GLU	B	631	26.454	44.100	86.881	1.00	8.28	B	C
ATOM	2503	CB	GLU	B	631	26.065	45.421	87.591	1.00	8.34	B	C
ATOM	2504	CG	GLU	B	631	27.245	46.390	87.867	1.00	8.93	B	C
ATOM	2505	CD	GLU	B	631	26.927	47.495	88.891	1.00	8.64	B	C
ATOM	2506	OE1	GLU	B	631	26.399	47.178	89.979	1.00	9.42	B	O
ATOM	2507	OE2	GLU	B	631	27.223	48.680	88.619	1.00	7.18	B	O
ATOM	2508	C	GLU	B	631	27.200	43.143	87.841	1.00	8.41	B	C
ATOM	2509	O	GLU	B	631	28.399	43.309	88.106	1.00	8.53	B	O
ATOM	2510	N	GLN	B	632	26.488	42.141	88.356	1.00	7.89	B	N
ATOM	2511	CA	GLN	B	632	27.102	41.164	89.247	1.00	7.38	B	C
ATOM	2512	CB	GLN	B	632	26.040	40.471	90.110	1.00	5.66	B	C
ATOM	2513	CG	GLN	B	632	25.503	41.335	91.243	1.00	3.17	B	C
ATOM	2514	CD	GLN	B	632	26.003	40.911	92.613	1.00	1.69	B	C
ATOM	2515	OE1	GLN	B	632	27.180	40.606	92.797	1.00	0.31	B	O
ATOM	2516	NE2	GLN	B	632	25.108	40.907	93.584	1.00	0.00	B	N
ATOM	2517	C	GLN	B	632	27.857	40.134	88.406	1.00	7.89	B	C
ATOM	2518	O	GLN	B	632	28.508	39.232	88.943	1.00	9.09	B	O
ATOM	2519	N	ARG	B	633	27.773	40.288	87.086	1.00	7.91	B	N
ATOM	2520	CA	ARG	B	633	28.446	39.396	86.155	1.00	8.24	B	C
ATOM	2521	CB	ARG	B	633	27.442	38.810	85.166	1.00	9.11	B	C
ATOM	2522	CG	ARG	B	633	27.994	37.683	84.286	1.00	8.31	B	C
ATOM	2523	CD	ARG	B	633	26.849	36.800	83.848	1.00	8.44	B	C
ATOM	2524	NE	ARG	B	633	26.017	36.501	85.007	1.00	9.93	B	N
ATOM	2525	CZ	ARG	B	633	24.720	36.250	84.958	1.00	8.99	B	C
ATOM	2526	NH1	ARG	B	633	24.083	36.253	83.796	1.00	9.55	B	N
ATOM	2527	NH2	ARG	B	633	24.062	36.022	86.082	1.00	8.74	B	N
ATOM	2528	C	ARG	B	633	29.528	40.159	85.402	1.00	8.55	B	C
ATOM	2529	O	ARG	B	633	30.053	39.696	84.392	1.00	8.86	B	O
ATOM	2530	N	MET	B	634	29.847	41.348	85.883	1.00	9.45	B	N
ATOM	2531	CA	MET	B	634	30.890	42.148	85.259	1.00	9.98	B	C
ATOM	2532	CB	MET	B	634	30.449	43.610	85.179	1.00	10.92	B	C
ATOM	2533	CG	MET	B	634	28.985	43.776	84.805	1.00	11.55	B	C
ATOM	2534	SD	MET	B	634	28.404	45.495	84.954	1.00	12.74	B	S
ATOM	2535	CE	MET	B	634	28.352	45.990	83.191	1.00	12.39	B	C
ATOM	2536	C	MET	B	634	32.080	41.987	86.210	1.00	9.74	B	C
ATOM	2537	O	MET	B	634	32.933	42.881	86.355	1.00	9.15	B	O
ATOM	2538	N	THR	B	635	32.105	40.822	86.856	1.00	8.39	B	N
ATOM	2539	CA	THR	B	635	33.135	40.466	87.826	1.00	7.94	B	C
ATOM	2540	CB	THR	B	635	32.527	40.326	89.221	1.00	9.56	B	C
ATOM	2541	OG1	THR	B	635	31.913	39.031	89.346	1.00	8.57	B	O
ATOM	2542	CG2	THR	B	635	31.458	41.423	89.438	1.00	10.40	B	C
ATOM	2543	C	THR	B	635	33.730	39.124	87.450	1.00	6.48	B	C
ATOM	2544	O	THR	B	635	34.939	38.921	87.483	1.00	6.42	B	O
ATOM	2545	N	LEU	B	636	32.835	38.218	87.081	1.00	6.45	B	N
ATOM	2546	CA	LEU	B	636	33.171	36.865	86.674	1.00	6.37	B	C
ATOM	2547	CB	LEU	B	636	31.881	36.016	86.667	1.00	3.85	B	C
ATOM	2548	CG	LEU	B	636	31.824	34.520	86.326	1.00	2.48	B	C
ATOM	2549	CD1	LEU	B	636	30.575	33.864	86.918	1.00	1.29	B	C
ATOM	2550	CD2	LEU	B	636	31.820	34.354	84.823	1.00	1.98	B	C
ATOM	2551	C	LEU	B	636	33.881	36.818	85.313	1.00	8.32	B	C
ATOM	2552	O	LEU	B	636	34.310	35.745	84.882	1.00	7.96	B	O
ATOM	2553	N	PRO	B	637	34.051	37.976	84.624	1.00	9.88	B	N
ATOM	2554	CD	PRO	B	637	33.519	39.352	84.713	1.00	9.39	B	C

ATOM	2555	CA	PRO	B	637	34.738	37.802	83.342	1.00	11.05	B	C
ATOM	2556	CB	PRO	B	637	34.265	39.017	82.534	1.00	9.72	B	C
ATOM	2557	CG	PRO	B	637	34.217	40.062	83.559	1.00	8.64	B	C
ATOM	2558	C	PRO	B	637	36.270	37.703	83.403	1.00	13.46	B	C
ATOM	2559	O	PRO	B	637	36.938	38.359	84.217	1.00	14.90	B	O
ATOM	2560	N	ASP	B	638	36.813	36.855	82.534	1.00	13.65	B	N
ATOM	2561	CA	ASP	B	638	38.254	36.694	82.402	1.00	12.96	B	C
ATOM	2562	CB	ASP	B	638	38.560	35.536	81.436	1.00	13.27	B	C
ATOM	2563	CG	ASP	B	638	40.009	35.084	81.485	1.00	11.66	B	C
ATOM	2564	OD1	ASP	B	638	40.908	35.947	81.430	1.00	9.78	B	O
ATOM	2565	OD2	ASP	B	638	40.243	33.855	81.567	1.00	9.98	B	O
ATOM	2566	C	ASP	B	638	38.623	38.039	81.760	1.00	13.79	B	C
ATOM	2567	O	ASP	B	638	39.720	38.209	81.227	1.00	18.18	B	O
ATOM	2568	N	MET	B	639	37.655	38.965	81.794	1.00	12.76	B	N
ATOM	2569	CA	MET	B	639	37.776	40.332	81.274	1.00	12.47	B	C
ATOM	2570	CB	MET	B	639	37.490	40.403	79.758	1.00	14.50	B	C
ATOM	2571	CG	MET	B	639	37.407	41.850	79.200	1.00	10.67	B	C
ATOM	2572	SD	MET	B	639	37.606	42.030	77.393	1.00	7.70	B	S
ATOM	2573	CE	MET	B	639	36.034	42.793	76.868	1.00	5.74	B	C
ATOM	2574	C	MET	B	639	36.862	41.337	81.998	1.00	12.93	B	C
ATOM	2575	O	MET	B	639	35.706	41.577	81.607	1.00	12.98	B	O
ATOM	2576	N	TYR	B	640	37.400	41.903	83.072	1.00	11.95	B	N
ATOM	2577	CA	TYR	B	640	36.721	42.920	83.862	1.00	9.67	B	C
ATOM	2578	CB	TYR	B	640	36.394	42.397	85.251	1.00	6.77	B	C
ATOM	2579	CG	TYR	B	640	36.375	43.474	86.285	1.00	5.87	B	C
ATOM	2580	CD1	TYR	B	640	35.357	44.422	86.319	1.00	5.63	B	C
ATOM	2581	CE1	TYR	B	640	35.378	45.463	87.244	1.00	5.53	B	C
ATOM	2582	CD2	TYR	B	640	37.413	43.589	87.203	1.00	6.07	B	C
ATOM	2583	CE2	TYR	B	640	37.438	44.630	88.132	1.00	5.83	B	C
ATOM	2584	CZ	TYR	B	640	36.419	45.553	88.144	1.00	4.97	B	C
ATOM	2585	OH	TYR	B	640	36.433	46.536	89.087	1.00	6.67	B	O
ATOM	2586	C	TYR	B	640	37.806	43.983	83.917	1.00	8.84	B	C
ATOM	2587	O	TYR	B	640	37.589	45.142	84.281	1.00	7.07	B	O
ATOM	2588	N	ASP	B	641	38.997	43.537	83.535	1.00	9.04	B	N
ATOM	2589	CA	ASP	B	641	40.164	44.395	83.449	1.00	8.79	B	C
ATOM	2590	CB	ASP	B	641	41.456	43.553	83.507	1.00	8.34	B	C
ATOM	2591	CG	ASP	B	641	41.199	42.058	83.354	1.00	5.99	B	C
ATOM	2592	OD1	ASP	B	641	40.357	41.515	84.101	1.00	4.95	B	O
ATOM	2593	OD2	ASP	B	641	41.851	41.425	82.498	1.00	3.33	B	O
ATOM	2594	C	ASP	B	641	39.998	45.073	82.081	1.00	9.57	B	C
ATOM	2595	O	ASP	B	641	40.854	45.830	81.613	1.00	10.91	B	O
ATOM	2596	N	GLN	B	642	38.864	44.775	81.456	1.00	9.01	B	N
ATOM	2597	CA	GLN	B	642	38.503	45.324	80.161	1.00	8.20	B	C
ATOM	2598	CB	GLN	B	642	39.498	44.841	79.077	1.00	7.93	B	C
ATOM	2599	CG	GLN	B	642	40.607	45.867	78.783	1.00	4.06	B	C
ATOM	2600	CD	GLN	B	642	42.041	45.299	78.810	1.00	3.80	B	C
ATOM	2601	OE1	GLN	B	642	42.466	44.650	79.779	1.00	3.12	B	O
ATOM	2602	NE2	GLN	B	642	42.798	45.569	77.746	1.00	2.28	B	N
ATOM	2603	C	GLN	B	642	37.028	44.965	79.846	1.00	8.23	B	C
ATOM	2604	O	GLN	B	642	36.684	44.394	78.808	1.00	6.78	B	O
ATOM	2605	N	CYS	B	643	36.162	45.322	80.787	1.00	8.29	B	N
ATOM	2606	CA	CYS	B	643	34.730	45.098	80.667	1.00	8.60	B	C
ATOM	2607	CB	CYS	B	643	34.258	44.133	81.738	1.00	9.67	B	C
ATOM	2608	SG	CYS	B	643	34.173	44.954	83.341	1.00	14.21	B	S
ATOM	2609	C	CYS	B	643	34.141	46.462	80.970	1.00	7.46	B	C
ATOM	2610	O	CYS	B	643	32.956	46.720	80.771	1.00	6.22	B	O
ATOM	2611	N	LYS	B	644	35.012	47.320	81.482	1.00	7.31	B	N
ATOM	2612	CA	LYS	B	644	34.662	48.675	81.860	1.00	7.34	B	C
ATOM	2613	CB	LYS	B	644	35.510	49.121	83.053	1.00	10.71	B	C
ATOM	2614	CG	LYS	B	644	37.012	48.911	82.853	1.00	12.57	B	C
ATOM	2615	CD	LYS	B	644	37.818	49.281	84.103	1.00	15.15	B	C
ATOM	2616	CE	LYS	B	644	39.305	48.942	83.958	1.00	16.34	B	C
ATOM	2617	NZ	LYS	B	644	39.923	49.549	82.740	1.00	17.09	B	N
ATOM	2618	C	LYS	B	644	34.893	49.621	80.708	1.00	6.16	B	C
ATOM	2619	O	LYS	B	644	34.139	50.564	80.515	1.00	6.91	B	O
ATOM	2620	N	HIS	B	645	35.937	49.384	79.933	1.00	3.96	B	N
ATOM	2621	CA	HIS	B	645	36.200	50.275	78.827	1.00	2.33	B	C
ATOM	2622	CB	HIS	B	645	37.317	49.704	77.963	1.00	1.18	B	C
ATOM	2623	CG	HIS	B	645	38.631	49.654	78.672	1.00	0.99	B	C
ATOM	2624	CD2	HIS	B	645	38.972	50.038	79.925	1.00	0.48	B	C
ATOM	2625	ND1	HIS	B	645	39.780	49.170	78.090	1.00	0.21	B	N
ATOM	2626	CE1	HIS	B	645	40.776	49.258	78.957	1.00	0.22	B	C
ATOM	2627	NE2	HIS	B	645	40.311	49.780	80.076	1.00	0.00	B	N
ATOM	2628	C	HIS	B	645	34.939	50.533	78.023	1.00	1.30	B	C
ATOM	2629	O	HIS	B	645	34.488	51.663	77.908	1.00	0.82	B	O
ATOM	2630	N	MET	B	646	34.345	49.478	77.497	1.00	0.56	B	N
ATOM	2631	CA	MET	B	646	33.146	49.633	76.711	1.00	0.00	B	C
ATOM	2632	CB	MET	B	646	32.638	48.280	76.284	1.00	0.00	B	C
ATOM	2633	CG	MET	B	646	33.687	47.370	75.720	1.00	1.32	B	C
ATOM	2634	SD	MET	B	646	32.848	45.897	75.157	1.00	4.15	B	S
ATOM	2635	CE	MET	B	646	31.833	45.515	76.587	1.00	4.12	B	C

ATOM	2636	C	MET	B	646	32.057	50.341	77.491	1.00	0.00	B	C
ATOM	2637	O	MET	B	646	31.299	51.111	76.925	1.00	0.00	B	O
ATOM	2638	N	LEU	B	647	31.958	50.065	78.786	1.00	0.00	B	N
ATOM	2639	CA	LEU	B	647	30.939	50.702	79.624	1.00	0.00	B	C
ATOM	2640	CB	LEU	B	647	30.842	49.964	80.957	1.00	0.00	B	C
ATOM	2641	CG	LEU	B	647	29.543	50.132	81.722	1.00	0.00	B	C
ATOM	2642	CD1	LEU	B	647	28.416	49.541	80.923	1.00	0.00	B	C
ATOM	2643	CD2	LEU	B	647	29.648	49.462	83.055	1.00	0.00	B	C
ATOM	2644	C	LEU	B	647	31.300	52.183	79.844	1.00	1.27	B	C
ATOM	2645	O	LEU	B	647	30.428	53.048	79.946	1.00	0.00	B	O
ATOM	2646	N	TYR	B	648	32.603	52.451	79.906	1.00	3.34	B	N
ATOM	2647	CA	TYR	B	648	33.152	53.797	80.070	1.00	4.93	B	C
ATOM	2648	CB	TYR	B	648	34.681	53.746	80.204	1.00	2.83	B	C
ATOM	2649	CG	TYR	B	648	35.236	53.570	81.602	1.00	4.48	B	C
ATOM	2650	CD1	TYR	B	648	36.596	53.354	81.792	1.00	4.35	B	C
ATOM	2651	CE1	TYR	B	648	37.131	53.228	83.055	1.00	4.34	B	C
ATOM	2652	CD2	TYR	B	648	34.414	53.653	82.732	1.00	4.68	B	C
ATOM	2653	CE2	TYR	B	648	34.941	53.528	84.014	1.00	3.46	B	C
ATOM	2654	CZ	TYR	B	648	36.305	53.317	84.161	1.00	4.16	B	C
ATOM	2655	OH	TYR	B	648	36.862	53.199	85.409	1.00	5.17	B	O
ATOM	2656	C	TYR	B	648	32.825	54.593	78.809	1.00	5.48	B	C
ATOM	2657	O	TYR	B	648	33.408	55.665	78.569	1.00	7.80	B	O
ATOM	2658	N	VAL	B	649	31.914	54.047	77.999	1.00	4.36	B	N
ATOM	2659	CA	VAL	B	649	31.493	54.667	76.745	1.00	2.80	B	C
ATOM	2660	CB	VAL	B	649	31.495	53.657	75.596	1.00	2.04	B	C
ATOM	2661	CG1	VAL	B	649	30.963	54.308	74.346	1.00	1.75	B	C
ATOM	2662	CG2	VAL	B	649	32.899	53.114	75.374	1.00	2.10	B	C
ATOM	2663	C	VAL	B	649	30.081	55.186	76.882	1.00	2.51	B	C
ATOM	2664	O	VAL	B	649	29.735	56.235	76.361	1.00	0.00	B	O
ATOM	2665	N	SER	B	650	29.267	54.433	77.602	1.00	3.61	B	N
ATOM	2666	CA	SER	B	650	27.879	54.800	77.800	1.00	4.00	B	C
ATOM	2667	CB	SER	B	650	27.074	53.548	78.129	1.00	3.75	B	C
ATOM	2668	OG	SER	B	650	27.726	52.813	79.150	1.00	6.70	B	O
ATOM	2669	C	SER	B	650	27.669	55.849	78.883	1.00	3.42	B	C
ATOM	2670	O	SER	B	650	26.536	56.221	79.156	1.00	3.44	B	O
ATOM	2671	N	SER	B	651	28.744	56.326	79.503	1.00	2.15	B	N
ATOM	2672	CA	SER	B	651	28.608	57.339	80.553	1.00	1.27	B	C
ATOM	2673	CB	SER	B	651	29.289	56.869	81.845	1.00	1.99	B	C
ATOM	2674	OG	SER	B	651	28.384	56.187	82.694	1.00	0.00	B	O
ATOM	2675	C	SER	B	651	29.107	58.739	80.182	1.00	0.88	B	C
ATOM	2676	O	SER	B	651	28.987	59.670	80.967	1.00	1.76	B	O
ATOM	2677	N	GLU	B	652	29.663	58.884	78.989	1.00	0.00	B	N
ATOM	2678	CA	GLU	B	652	30.141	60.173	78.524	1.00	0.00	B	C
ATOM	2679	CB	GLU	B	652	31.635	60.083	78.163	1.00	0.00	B	C
ATOM	2680	CG	GLU	B	652	32.348	61.422	77.974	1.00	0.00	B	C
ATOM	2681	CD	GLU	B	652	32.113	62.376	79.133	1.00	0.00	B	C
ATOM	2682	OE1	GLU	B	652	32.374	61.967	80.284	1.00	0.00	B	O
ATOM	2683	OE2	GLU	B	652	31.669	63.529	78.886	1.00	0.00	B	O
ATOM	2684	C	GLU	B	652	29.272	60.457	77.302	1.00	0.00	B	C
ATOM	2685	O	GLU	B	652	29.281	61.532	76.737	1.00	0.00	B	O
ATOM	2686	N	LEU	B	653	28.520	59.442	76.913	1.00	0.00	B	N
ATOM	2687	CA	LEU	B	653	27.585	59.494	75.802	1.00	0.00	B	C
ATOM	2688	CB	LEU	B	653	27.459	58.088	75.192	1.00	0.11	B	C
ATOM	2689	CG	LEU	B	653	26.801	57.694	73.861	1.00	0.00	B	C
ATOM	2690	CD1	LEU	B	653	25.425	58.282	73.772	1.00	1.46	B	C
ATOM	2691	CD2	LEU	B	653	27.644	58.148	72.698	1.00	0.75	B	C
ATOM	2692	C	LEU	B	653	26.306	59.869	76.550	1.00	0.00	B	C
ATOM	2693	O	LEU	B	653	25.320	60.308	75.981	1.00	0.00	B	O
ATOM	2694	N	HIS	B	654	26.349	59.691	77.860	1.00	0.00	B	N
ATOM	2695	CA	HIS	B	654	25.220	59.993	78.713	1.00	0.30	B	C
ATOM	2696	CB	HIS	B	654	24.969	58.829	79.649	1.00	0.00	B	C
ATOM	2697	CG	HIS	B	654	23.757	58.989	80.505	1.00	0.03	B	C
ATOM	2698	CD2	HIS	B	654	22.495	58.530	80.353	1.00	0.00	B	C
ATOM	2699	ND1	HIS	B	654	23.777	59.676	81.697	1.00	0.86	B	N
ATOM	2700	CE1	HIS	B	654	22.578	59.628	82.245	1.00	0.86	B	C
ATOM	2701	NE2	HIS	B	654	21.782	58.938	81.451	1.00	0.22	B	N
ATOM	2702	C	HIS	B	654	25.561	61.226	79.504	1.00	0.89	B	C
ATOM	2703	O	HIS	B	654	24.672	61.944	79.974	1.00	1.36	B	O
ATOM	2704	N	ARG	B	655	26.865	61.449	79.668	1.00	1.35	B	N
ATOM	2705	CA	ARG	B	655	27.363	62.620	80.373	1.00	2.84	B	C
ATOM	2706	CB	ARG	B	655	28.885	62.547	80.525	1.00	3.77	B	C
ATOM	2707	CG	ARG	B	655	29.555	63.879	80.817	1.00	5.23	B	C
ATOM	2708	CD	ARG	B	655	30.802	63.753	81.707	1.00	7.20	B	C
ATOM	2709	NE	ARG	B	655	30.481	63.586	83.130	1.00	7.25	B	N
ATOM	2710	CZ	ARG	B	655	31.271	63.967	84.134	1.00	7.26	B	C
ATOM	2711	NH1	ARG	B	655	32.437	64.540	83.886	1.00	8.16	B	N
ATOM	2712	NH2	ARG	B	655	30.887	63.786	85.390	1.00	7.43	B	N
ATOM	2713	C	ARG	B	655	26.963	63.781	79.483	1.00	3.12	B	C
ATOM	2714	O	ARG	B	655	26.332	64.730	79.934	1.00	3.47	B	O
ATOM	2715	N	LEU	B	656	27.304	63.676	78.202	1.00	2.73	B	N
ATOM	2716	CA	LEU	B	656	26.956	64.705	77.231	1.00	2.39	B	C

ATOM	2717	CB	LEU	B	656	27.909	64.682	76.033	1.00	0.24	B	C
ATOM	2718	CG	LEU	B	656	29.398	64.888	76.301	1.00	0.00	B	C
ATOM	2719	CD1	LEU	B	656	30.161	64.929	74.988	1.00	0.00	B	C
ATOM	2720	CD2	LEU	B	656	29.586	66.166	77.061	1.00	0.00	B	C
ATOM	2721	C	LEU	B	656	25.536	64.504	76.725	1.00	3.19	B	C
ATOM	2722	O	LEU	B	656	25.124	65.161	75.774	1.00	3.40	B	O
ATOM	2723	N	GLN	B	657	24.795	63.592	77.352	1.00	3.85	B	N
ATOM	2724	CA	GLN	B	657	23.414	63.309	76.959	1.00	4.18	B	C
ATOM	2725	CB	GLN	B	657	22.454	64.231	77.720	1.00	6.48	B	C
ATOM	2726	CG	GLN	B	657	22.582	64.173	79.249	1.00	11.61	B	C
ATOM	2727	CD	GLN	B	657	21.694	65.195	79.978	1.00	13.93	B	C
ATOM	2728	OE1	GLN	B	657	21.753	65.322	81.203	1.00	15.56	B	O
ATOM	2729	NE2	GLN	B	657	20.872	65.921	79.224	1.00	14.40	B	N
ATOM	2730	C	GLN	B	657	23.174	63.461	75.447	1.00	2.89	B	C
ATOM	2731	O	GLN	B	657	22.112	63.913	75.027	1.00	1.31	B	O
ATOM	2732	N	VAL	B	658	24.171	63.078	74.648	1.00	1.74	B	N
ATOM	2733	CA	VAL	B	658	24.108	63.152	73.187	1.00	0.37	B	C
ATOM	2734	CB	VAL	B	658	25.131	62.205	72.532	1.00	0.72	B	C
ATOM	2735	CG1	VAL	B	658	25.122	62.386	71.023	1.00	2.31	B	C
ATOM	2736	CG2	VAL	B	658	26.505	62.472	73.085	1.00	0.94	B	C
ATOM	2737	C	VAL	B	658	22.746	62.746	72.697	1.00	0.00	B	C
ATOM	2738	O	VAL	B	658	22.013	62.085	73.409	1.00	0.00	B	O
ATOM	2739	N	SER	B	659	22.402	63.135	71.480	1.00	0.00	B	N
ATOM	2740	CA	SER	B	659	21.106	62.761	70.932	1.00	0.00	B	C
ATOM	2741	CB	SER	B	659	20.376	63.996	70.411	1.00	0.00	B	C
ATOM	2742	OG	SER	B	659	20.183	64.927	71.452	1.00	0.00	B	O
ATOM	2743	C	SER	B	659	21.219	61.724	69.817	1.00	2.02	B	C
ATOM	2744	O	SER	B	659	22.325	61.381	69.380	1.00	1.89	B	O
ATOM	2745	N	TYR	B	660	20.063	61.233	69.365	1.00	4.01	B	N
ATOM	2746	CA	TYR	B	660	19.980	60.236	68.291	1.00	4.74	B	C
ATOM	2747	CB	TYR	B	660	18.581	59.598	68.268	1.00	3.00	B	C
ATOM	2748	CG	TYR	B	660	18.411	58.536	67.212	1.00	0.00	B	C
ATOM	2749	CD1	TYR	B	660	18.831	57.230	67.436	1.00	0.00	B	C
ATOM	2750	CE1	TYR	B	660	18.707	56.259	66.453	1.00	0.00	B	C
ATOM	2751	CD2	TYR	B	660	17.860	58.847	65.972	1.00	0.00	B	C
ATOM	2752	CE2	TYR	B	660	17.735	57.886	64.979	1.00	0.00	B	C
ATOM	2753	CZ	TYR	B	660	18.159	56.593	65.228	1.00	0.00	B	C
ATOM	2754	OH	TYR	B	660	18.027	55.639	64.248	1.00	0.00	B	O
ATOM	2755	C	TYR	B	660	20.289	60.861	66.922	1.00	5.76	B	C
ATOM	2756	O	TYR	B	660	21.240	60.472	66.245	1.00	7.12	B	O
ATOM	2757	N	GLU	B	661	19.480	61.828	66.511	1.00	6.06	B	N
ATOM	2758	CA	GLU	B	661	19.712	62.492	65.242	1.00	6.44	B	C
ATOM	2759	CB	GLU	B	661	18.605	63.511	64.974	1.00	7.22	B	C
ATOM	2760	CG	GLU	B	661	17.193	63.023	65.346	1.00	8.43	B	C
ATOM	2761	CD	GLU	B	661	16.620	61.966	64.395	1.00	8.03	B	C
ATOM	2762	OE1	GLU	B	661	15.520	61.434	64.677	1.00	7.13	B	O
ATOM	2763	OE2	GLU	B	661	17.260	61.674	63.365	1.00	7.62	B	C
ATOM	2764	C	GLU	B	661	21.056	63.198	65.383	1.00	6.19	B	C
ATOM	2765	O	GLU	B	661	21.466	63.948	64.510	1.00	8.69	B	O
ATOM	2766	N	GLU	B	662	21.730	62.938	66.502	1.00	5.14	B	N
ATOM	2767	CA	GLU	B	662	23.032	63.517	66.829	1.00	4.36	B	C
ATOM	2768	CB	GLU	B	662	22.942	64.257	68.175	1.00	3.06	B	C
ATOM	2769	CG	GLU	B	662	24.143	65.127	68.564	1.00	2.11	B	C
ATOM	2770	CD	GLU	B	662	24.066	65.665	69.995	1.00	1.78	B	C
ATOM	2771	OE1	GLU	B	662	22.978	66.096	70.411	1.00	1.59	B	O
ATOM	2772	OE2	GLU	B	662	25.093	65.667	70.702	1.00	1.65	B	C
ATOM	2773	C	GLU	B	662	24.021	62.366	66.941	1.00	4.24	B	C
ATOM	2774	O	GLU	B	662	25.212	62.568	67.087	1.00	2.99	B	O
ATOM	2775	N	TYR	B	663	23.498	61.150	66.857	1.00	3.70	B	N
ATOM	2776	CA	TYR	B	663	24.281	59.913	66.958	1.00	1.87	B	C
ATOM	2777	CB	TYR	B	663	23.493	58.908	67.808	1.00	0.44	B	C
ATOM	2778	CG	TYR	B	663	23.786	57.446	67.550	1.00	1.17	B	C
ATOM	2779	CD1	TYR	B	663	24.986	56.866	67.955	1.00	0.80	B	C
ATOM	2780	CE1	TYR	B	663	25.242	55.515	67.742	1.00	1.25	B	C
ATOM	2781	CD2	TYR	B	663	22.849	56.637	66.921	1.00	0.76	B	C
ATOM	2782	CE2	TYR	B	663	23.095	55.285	66.700	1.00	0.42	B	C
ATOM	2783	CZ	TYR	B	663	24.292	54.730	67.113	1.00	1.11	B	C
ATOM	2784	OH	TYR	B	663	24.539	53.393	66.890	1.00	2.40	B	O
ATOM	2785	C	TYR	B	663	24.617	59.293	65.599	1.00	0.61	B	C
ATOM	2786	O	TYR	B	663	25.752	58.941	65.323	1.00	1.26	B	O
ATOM	2787	N	LEU	B	664	23.602	59.155	64.760	1.00	0.00	B	N
ATOM	2788	CA	LEU	B	664	23.763	58.576	63.441	1.00	0.00	B	C
ATOM	2789	CB	LEU	B	664	22.424	58.605	62.684	1.00	0.00	B	C
ATOM	2790	CG	LEU	B	664	21.084	58.254	63.350	1.00	0.00	B	C
ATOM	2791	CD1	LEU	B	664	19.986	58.340	62.321	1.00	0.00	B	C
ATOM	2792	CD2	LEU	B	664	21.126	56.869	63.937	1.00	0.00	B	C
ATOM	2793	C	LEU	B	664	24.812	59.343	62.650	1.00	0.00	B	C
ATOM	2794	O	LEU	B	664	25.354	58.827	61.686	1.00	0.24	B	O
ATOM	2795	N	CYS	B	665	25.083	60.585	63.043	1.00	0.00	B	N
ATOM	2796	CA	CYS	B	665	26.088	61.401	62.359	1.00	0.00	B	C
ATOM	2797	CB	CYS	B	665	25.741	62.876	62.439	1.00	0.00	B	C

ATOM	2798	SG	CYS	B	665	25.300	63.577	60.867	1.00	0.00	B	S
ATOM	2799	C	CYS	B	665	27.403	61.179	63.049	1.00	0.00	B	C
ATOM	2800	O	CYS	B	665	28.426	60.982	62.407	1.00	0.00	B	O
ATOM	2801	N	MET	B	666	27.351	61.205	64.375	1.00	0.03	B	N
ATOM	2802	CA	MET	B	666	28.524	60.993	65.204	1.00	0.67	B	C
ATOM	2803	CB	MET	B	666	28.115	60.976	66.674	1.00	0.00	B	C
ATOM	2804	CG	MET	B	666	29.207	61.363	67.639	1.00	0.46	B	C
ATOM	2805	SD	MET	B	666	28.527	62.015	69.191	1.00	0.00	B	S
ATOM	2806	CE	MET	B	666	28.221	60.528	70.092	1.00	0.57	B	C
ATOM	2807	C	MET	B	666	29.199	59.680	64.827	1.00	0.95	B	C
ATOM	2808	O	MET	B	666	30.391	59.657	64.561	1.00	1.95	B	O
ATOM	2809	N	LYS	B	667	28.439	58.590	64.778	1.00	0.40	B	N
ATOM	2810	CA	LYS	B	667	29.018	57.301	64.429	1.00	0.63	B	C
ATOM	2811	CB	LYS	B	667	28.019	56.163	64.562	1.00	2.57	B	C
ATOM	2812	CG	LYS	B	667	28.673	54.783	64.444	1.00	0.68	B	C
ATOM	2813	CD	LYS	B	667	27.653	53.705	64.244	1.00	0.32	B	C
ATOM	2814	CE	LYS	B	667	27.120	53.756	62.837	1.00	0.82	B	C
ATOM	2815	NZ	LYS	B	667	25.925	52.887	62.690	1.00	2.75	B	N
ATOM	2816	C	LYS	B	667	29.523	57.281	63.020	1.00	0.73	B	C
ATOM	2817	O	LYS	B	667	30.649	56.867	62.786	1.00	3.35	B	O
ATOM	2818	N	THR	B	668	28.691	57.701	62.075	1.00	0.09	B	N
ATOM	2819	CA	THR	B	668	29.104	57.712	60.676	1.00	0.00	B	C
ATOM	2820	CB	THR	B	668	28.080	58.432	59.797	1.00	0.00	B	C
ATOM	2821	OG1	THR	B	668	26.801	57.825	59.979	1.00	0.00	B	O
ATOM	2822	CG2	THR	B	668	28.460	58.320	58.325	1.00	0.00	B	C
ATOM	2823	C	THR	B	668	30.479	58.356	60.464	1.00	0.46	B	C
ATOM	2824	O	THR	B	668	31.006	58.355	59.350	1.00	0.63	B	O
ATOM	2825	N	LEU	B	669	31.050	58.903	61.536	1.00	0.09	B	N
ATOM	2826	CA	LEU	B	669	32.371	59.518	61.485	1.00	0.62	B	C
ATOM	2827	CB	LEU	B	669	32.363	60.865	62.211	1.00	0.00	B	C
ATOM	2828	CG	LEU	B	669	31.629	62.014	61.505	1.00	0.14	B	C
ATOM	2829	CD1	LEU	B	669	31.713	63.267	62.363	1.00	0.35	B	C
ATOM	2830	CD2	LEU	B	669	32.233	62.263	60.130	1.00	0.00	B	C
ATOM	2831	C	LEU	B	669	33.422	58.590	62.095	1.00	0.56	B	C
ATOM	2832	O	LEU	B	669	34.619	58.790	61.921	1.00	1.08	B	O
ATOM	2833	N	LEU	B	670	32.980	57.577	62.825	1.00	1.32	B	N
ATOM	2834	CA	LEU	B	670	33.925	56.639	63.386	1.00	2.02	B	C
ATOM	2835	CB	LEU	B	670	33.261	55.732	64.415	1.00	2.40	B	C
ATOM	2836	CG	LEU	B	670	33.204	56.317	65.823	1.00	2.85	B	C
ATOM	2837	CD1	LEU	B	670	32.685	55.276	66.792	1.00	2.27	B	C
ATOM	2838	CD2	LEU	B	670	34.588	56.777	66.246	1.00	2.47	B	C
ATOM	2839	C	LEU	B	670	34.475	55.810	62.237	1.00	2.95	B	C
ATOM	2840	O	LEU	B	670	35.564	55.245	62.340	1.00	3.88	B	O
ATOM	2841	N	LEU	B	671	33.721	55.740	61.140	1.00	3.57	B	N
ATOM	2842	CA	LEU	B	671	34.161	54.987	59.972	1.00	4.54	B	C
ATOM	2843	CB	LEU	B	671	33.036	54.840	58.955	1.00	4.10	B	C
ATOM	2844	CG	LEU	B	671	33.498	54.188	57.642	1.00	5.62	B	C
ATOM	2845	CD1	LEU	B	671	32.300	53.549	56.940	1.00	5.52	B	C
ATOM	2846	CD2	LEU	B	671	34.205	55.215	56.743	1.00	4.90	B	C
ATOM	2847	C	LEU	B	671	35.312	55.701	59.304	1.00	5.01	B	C
ATOM	2848	O	LEU	B	671	36.373	55.115	59.061	1.00	3.26	B	O
ATOM	2849	N	LEU	B	672	35.067	56.973	58.992	1.00	5.62	B	N
ATOM	2850	CA	LEU	B	672	36.037	57.853	58.342	1.00	3.54	B	C
ATOM	2851	CB	LEU	B	672	35.385	59.195	58.025	1.00	1.02	B	C
ATOM	2852	CG	LEU	B	672	34.143	59.180	57.146	1.00	2.07	B	C
ATOM	2853	CD1	LEU	B	672	33.586	60.596	57.067	1.00	1.51	B	C
ATOM	2854	CD2	LEU	B	672	34.487	58.641	55.761	1.00	2.88	B	C
ATOM	2855	C	LEU	B	672	37.268	58.109	59.198	1.00	2.14	B	C
ATOM	2856	O	LEU	B	672	38.389	58.056	58.722	1.00	1.65	B	O
ATOM	2857	N	SER	B	673	37.050	58.387	60.469	1.00	0.24	B	N
ATOM	2858	CA	SER	B	673	38.149	58.677	61.352	1.00	0.51	B	C
ATOM	2859	CB	SER	B	673	37.621	58.994	62.754	1.00	4.12	B	C
ATOM	2860	OG	SER	B	673	36.965	60.253	62.800	1.00	5.79	B	O
ATOM	2861	C	SER	B	673	39.225	57.606	61.428	1.00	0.36	B	C
ATOM	2862	O	SER	B	673	39.317	56.873	62.418	1.00	2.38	B	O
ATOM	2863	N	SER	B	674	40.039	57.538	60.375	1.00	0.22	B	N
ATOM	2864	CA	SER	B	674	41.180	56.619	60.239	1.00	0.08	B	C
ATOM	2865	CB	SER	B	674	40.922	55.253	60.891	1.00	0.00	B	C
ATOM	2866	OG	SER	B	674	41.776	55.056	62.011	1.00	0.00	B	O
ATOM	2867	C	SER	B	674	41.480	56.446	58.759	1.00	0.13	B	C
ATOM	2868	O	SER	B	674	40.626	56.017	57.989	1.00	0.00	B	O
ATOM	2869	N	VAL	B	675	42.698	56.809	58.370	1.00	0.96	B	N
ATOM	2870	CA	VAL	B	675	43.151	56.728	56.984	1.00	2.58	B	C
ATOM	2871	CB	VAL	B	675	43.304	58.133	56.382	1.00	4.64	B	C
ATOM	2872	CG1	VAL	B	675	43.120	58.095	54.873	1.00	6.17	B	C
ATOM	2873	CG2	VAL	B	675	42.334	59.082	57.052	1.00	7.58	B	C
ATOM	2874	C	VAL	B	675	44.534	56.100	56.974	1.00	1.31	B	C
ATOM	2875	O	VAL	B	675	45.200	56.042	58.004	1.00	3.84	B	O
ATOM	2876	N	PRO	B	676	44.980	55.591	55.822	1.00	0.53	B	N
ATOM	2877	CD	PRO	B	676	44.262	55.052	54.657	1.00	0.00	B	C
ATOM	2878	CA	PRO	B	676	46.326	55.025	55.900	1.00	0.02	B	C

ATOM	2879	CB	PRO	B	676	46.426	54.191	54.623	1.00	0.25	B	C
ATOM	2880	CG	PRO	B	676	45.017	53.767	54.389	1.00	0.00	B	C
ATOM	2881	C	PRO	B	676	47.269	56.222	55.896	1.00	0.38	B	C
ATOM	2882	O	PRO	B	676	47.073	57.157	55.129	1.00	0.00	B	O
ATOM	2883	N	LYS	B	677	48.272	56.203	56.766	1.00	2.40	B	N
ATOM	2884	CA	LYS	B	677	49.228	57.302	56.855	1.00	3.88	B	C
ATOM	2885	CB	LYS	B	677	50.481	56.864	57.616	1.00	2.58	B	C
ATOM	2886	CG	LYS	B	677	51.216	57.970	58.354	1.00	2.90	B	C
ATOM	2887	CD	LYS	B	677	52.129	57.384	59.445	1.00	1.94	B	C
ATOM	2888	CE	LYS	B	677	53.421	56.836	58.893	1.00	1.20	B	C
ATOM	2889	NZ	LYS	B	677	53.194	56.035	57.676	1.00	1.15	B	N
ATOM	2890	C	LYS	B	677	49.585	57.719	55.446	1.00	4.91	B	C
ATOM	2891	O	LYS	B	677	50.097	58.803	55.226	1.00	5.06	B	O
ATOM	2892	N	ASP	B	678	49.331	56.836	54.492	1.00	6.47	B	N
ATOM	2893	CA	ASP	B	678	49.570	57.152	53.102	1.00	8.82	B	C
ATOM	2894	CB	ASP	B	678	49.808	55.888	52.281	1.00	9.66	B	C
ATOM	2895	CG	ASP	B	678	51.142	55.255	52.576	1.00	10.29	B	C
ATOM	2896	OD1	ASP	B	678	52.171	55.945	52.410	1.00	9.32	B	O
ATOM	2897	OD2	ASP	B	678	51.158	54.074	52.978	1.00	10.07	B	O
ATOM	2898	C	ASP	B	678	48.267	57.812	52.708	1.00	9.42	B	C
ATOM	2899	O	ASP	B	678	47.857	58.755	53.363	1.00	11.73	B	O
ATOM	2900	N	GLY	B	679	47.595	57.322	51.673	1.00	9.36	B	N
ATOM	2901	CA	GLY	B	679	46.345	57.941	51.279	1.00	8.28	B	C
ATOM	2902	C	GLY	B	679	45.522	57.086	50.347	1.00	8.41	B	C
ATOM	2903	O	GLY	B	679	46.001	56.670	49.296	1.00	8.68	B	O
ATOM	2904	N	LEU	B	680	44.279	56.820	50.729	1.00	7.98	B	N
ATOM	2905	CA	LEU	B	680	43.385	56.010	49.913	1.00	7.83	B	C
ATOM	2906	CB	LEU	B	680	41.935	56.215	50.365	1.00	4.74	B	C
ATOM	2907	CG	LEU	B	680	41.623	56.333	51.861	1.00	4.65	B	C
ATOM	2908	CD1	LEU	B	680	40.157	56.660	52.056	1.00	4.10	B	C
ATOM	2909	CD2	LEU	B	680	41.973	55.048	52.563	1.00	3.63	B	C
ATOM	2910	C	LEU	B	680	43.522	56.445	48.452	1.00	7.74	B	C
ATOM	2911	O	LEU	B	680	43.769	57.619	48.177	1.00	7.99	B	O
ATOM	2912	N	LYS	B	681	43.373	55.512	47.515	1.00	7.37	B	N
ATOM	2913	CA	LYS	B	681	43.465	55.862	46.102	1.00	5.39	B	C
ATOM	2914	CB	LYS	B	681	43.361	54.619	45.214	1.00	3.99	B	C
ATOM	2915	CG	LYS	B	681	44.701	53.950	44.891	1.00	3.05	B	C
ATOM	2916	CD	LYS	B	681	45.104	52.902	45.924	1.00	1.07	B	C
ATOM	2917	CE	LYS	B	681	44.229	51.667	45.820	1.00	0.00	B	C
ATOM	2918	NZ	LYS	B	681	44.242	51.147	44.431	1.00	0.00	B	N
ATOM	2919	C	LYS	B	681	42.345	56.819	45.730	1.00	4.35	B	C
ATOM	2920	O	LYS	B	681	42.131	57.098	44.556	1.00	5.24	B	O
ATOM	2921	N	SER	B	682	41.625	57.319	46.727	1.00	2.35	B	N
ATOM	2922	CA	SER	B	682	40.528	58.233	46.470	1.00	1.78	B	C
ATOM	2923	CB	SER	B	682	39.201	57.482	46.520	1.00	1.42	B	C
ATOM	2924	OG	SER	B	682	39.288	56.225	45.882	1.00	0.00	B	O
ATOM	2925	C	SER	B	682	40.499	59.349	47.491	1.00	2.31	B	C
ATOM	2926	O	SER	B	682	39.452	59.927	47.743	1.00	2.40	B	O
ATOM	2927	N	GLN	B	683	41.647	59.645	48.086	1.00	2.71	B	N
ATOM	2928	CA	GLN	B	683	41.743	60.696	49.095	1.00	2.35	B	C
ATOM	2929	CB	GLN	B	683	43.212	61.071	49.319	1.00	0.39	B	C
ATOM	2930	CG	GLN	B	683	43.466	61.927	50.536	1.00	0.26	B	C
ATOM	2931	CD	GLN	B	683	43.122	61.208	51.822	1.00	1.21	B	C
ATOM	2932	OE1	GLN	B	683	43.237	61.771	52.910	1.00	0.85	B	O
ATOM	2933	NE2	GLN	B	683	42.703	59.955	51.709	1.00	0.24	B	N
ATOM	2934	C	GLN	B	683	40.944	61.945	48.695	1.00	2.85	B	C
ATOM	2935	O	GLN	B	683	40.115	62.436	49.466	1.00	2.53	B	O
ATOM	2936	N	GLU	B	684	41.201	62.454	47.489	1.00	2.97	B	N
ATOM	2937	CA	GLU	B	684	40.522	63.642	46.977	1.00	3.54	B	C
ATOM	2938	CB	GLU	B	684	40.710	63.741	45.467	1.00	3.41	B	C
ATOM	2939	CG	GLU	B	684	42.167	63.800	45.049	1.00	6.29	B	C
ATOM	2940	CD	GLU	B	684	42.434	63.049	43.754	1.00	7.77	B	C
ATOM	2941	OE1	GLU	B	684	41.998	61.876	43.651	1.00	7.69	B	O
ATOM	2942	OE2	GLU	B	684	43.086	63.622	42.850	1.00	8.64	B	O
ATOM	2943	C	GLU	B	684	39.058	63.499	47.307	1.00	4.17	B	C
ATOM	2944	O	GLU	B	684	38.448	64.381	47.907	1.00	2.88	B	O
ATOM	2945	N	LEU	B	685	38.496	62.367	46.913	1.00	6.54	B	N
ATOM	2946	CA	LEU	B	685	37.102	62.104	47.203	1.00	8.85	B	C
ATOM	2947	CB	LEU	B	685	36.667	60.739	46.641	1.00	11.58	B	C
ATOM	2948	CG	LEU	B	685	36.469	60.597	45.118	1.00	14.23	B	C
ATOM	2949	CD1	LEU	B	685	37.813	60.677	44.385	1.00	15.68	B	C
ATOM	2950	CD2	LEU	B	685	35.786	59.261	44.818	1.00	16.24	B	C
ATOM	2951	C	LEU	B	685	36.952	62.135	48.719	1.00	8.93	B	C
ATOM	2952	O	LEU	B	685	36.509	63.143	49.269	1.00	8.87	B	O
ATOM	2953	N	PHE	B	686	37.352	61.055	49.388	1.00	8.24	B	N
ATOM	2954	CA	PHE	B	686	37.240	60.964	50.842	1.00	7.97	B	C
ATOM	2955	CB	PHE	B	686	38.464	60.268	51.430	1.00	8.03	B	C
ATOM	2956	CG	PHE	B	686	38.525	60.342	52.929	1.00	8.39	B	C
ATOM	2957	CD1	PHE	B	686	37.489	59.840	53.705	1.00	8.30	B	C
ATOM	2958	CD2	PHE	B	686	39.602	60.941	53.566	1.00	8.77	B	C
ATOM	2959	CE1	PHE	B	686	37.524	59.933	55.088	1.00	8.53	B	C

ATOM	2960	CE2	PHE	B	686	39.644	61.038	54.959	1.00	8.39	B	C
ATOM	2961	CZ	PHE	B	686	38.606	60.534	55.717	1.00	8.56	B	C
ATOM	2962	C	PHE	B	686	37.024	62.303	51.576	1.00	7.17	B	C
ATOM	2963	O	PHE	B	686	36.071	62.450	52.355	1.00	6.33	B	O
ATOM	2964	N	ASP	B	687	37.915	63.265	51.330	1.00	6.64	B	N
ATOM	2965	CA	ASP	B	687	37.845	64.587	51.962	1.00	5.98	B	C
ATOM	2966	CB	ASP	B	687	38.769	65.591	51.248	1.00	6.99	B	C
ATOM	2967	CG	ASP	B	687	40.237	65.222	51.338	1.00	8.70	B	C
ATOM	2968	OD1	ASP	B	687	40.694	64.852	52.443	1.00	10.19	B	O
ATOM	2969	OD2	ASP	B	687	40.930	65.327	50.302	1.00	10.15	B	O
ATOM	2970	C	ASP	B	687	36.436	65.164	51.945	1.00	5.21	B	C
ATOM	2971	O	ASP	B	687	35.798	65.333	52.989	1.00	2.60	B	O
ATOM	2972	N	GLU	B	688	35.979	65.484	50.736	1.00	6.03	B	N
ATOM	2973	CA	GLU	B	688	34.665	66.065	50.522	1.00	5.79	B	C
ATOM	2974	CB	GLU	B	688	34.421	66.276	49.023	1.00	6.69	B	C
ATOM	2975	CG	GLU	B	688	34.959	65.150	48.165	1.00	9.91	B	C
ATOM	2976	CD	GLU	B	688	35.014	65.493	46.682	1.00	12.88	B	C
ATOM	2977	OE1	GLU	B	688	33.931	65.733	46.085	1.00	14.18	B	O
ATOM	2978	OE2	GLU	B	688	36.139	65.516	46.118	1.00	14.35	B	O
ATOM	2979	C	GLU	B	688	33.560	65.225	51.132	1.00	5.08	B	C
ATOM	2980	O	GLU	B	688	32.607	65.778	51.673	1.00	5.28	B	O
ATOM	2981	N	ILE	B	689	33.688	63.901	51.072	1.00	4.04	B	N
ATOM	2982	CA	ILE	B	689	32.660	63.036	51.634	1.00	5.68	B	C
ATOM	2983	CB	ILE	B	689	32.717	61.591	51.003	1.00	8.39	B	C
ATOM	2984	CG2	ILE	B	689	34.100	61.023	51.107	1.00	9.31	B	C
ATOM	2985	CG1	ILE	B	689	31.696	60.660	51.683	1.00	7.28	B	C
ATOM	2986	CD1	ILE	B	689	31.538	59.318	51.001	1.00	5.49	B	C
ATOM	2987	C	ILE	B	689	32.742	62.983	53.163	1.00	5.53	B	C
ATOM	2988	O	ILE	B	689	31.799	62.567	53.832	1.00	5.75	B	O
ATOM	2989	N	ARG	B	690	33.862	63.418	53.721	1.00	5.70	B	N
ATOM	2990	CA	ARG	B	690	34.008	63.430	55.172	1.00	5.67	B	C
ATOM	2991	CB	ARG	B	690	35.470	63.203	55.572	1.00	4.91	B	C
ATOM	2992	CG	ARG	B	690	35.798	63.596	57.013	1.00	3.32	B	C
ATOM	2993	CD	ARG	B	690	37.019	62.850	57.542	1.00	1.66	B	C
ATOM	2994	NE	ARG	B	690	37.494	63.386	58.812	1.00	0.00	B	N
ATOM	2995	CZ	ARG	B	690	38.290	64.444	58.918	1.00	0.00	B	C
ATOM	2996	NH1	ARG	B	690	38.710	65.078	57.831	1.00	0.00	B	N
ATOM	2997	NH2	ARG	B	690	38.656	64.873	60.116	1.00	0.00	B	N
ATOM	2998	C	ARG	B	690	33.526	64.769	55.710	1.00	6.61	B	C
ATOM	2999	O	ARG	B	690	32.605	64.831	56.530	1.00	6.73	B	C
ATOM	3000	N	MET	B	691	34.160	65.840	55.237	1.00	7.37	B	N
ATOM	3001	CA	MET	B	691	33.806	67.189	55.654	1.00	8.11	B	C
ATOM	3002	CB	MET	B	691	34.579	68.209	54.814	1.00	9.61	B	C
ATOM	3003	CG	MET	B	691	36.082	68.186	55.027	1.00	12.72	B	C
ATOM	3004	SD	MET	B	691	37.006	69.163	53.800	1.00	14.69	B	S
ATOM	3005	CE	MET	B	691	38.704	68.671	54.198	1.00	13.40	B	C
ATOM	3006	C	MET	B	691	32.301	67.399	55.489	1.00	7.30	B	C
ATOM	3007	O	MET	B	691	31.680	68.170	56.229	1.00	6.23	B	O
ATOM	3008	N	THR	B	692	31.725	66.681	54.526	1.00	7.04	B	N
ATOM	3009	CA	THR	B	692	30.302	66.770	54.229	1.00	7.48	B	C
ATOM	3010	CB	THR	B	692	29.999	66.380	52.779	1.00	8.38	B	C
ATOM	3011	OG1	THR	B	692	28.728	66.923	52.406	1.00	8.80	B	O
ATOM	3012	CG2	THR	B	692	29.937	64.849	52.628	1.00	9.23	B	C
ATOM	3013	C	THR	B	692	29.387	65.931	55.116	1.00	6.70	B	C
ATOM	3014	O	THR	B	692	28.237	65.694	54.772	1.00	8.46	B	O
ATOM	3015	N	TYR	B	693	29.893	65.443	56.234	1.00	5.22	B	N
ATOM	3016	CA	TYR	B	693	29.037	64.702	57.141	1.00	4.21	B	C
ATOM	3017	CB	TYR	B	693	29.514	63.256	57.339	1.00	3.29	B	C
ATOM	3018	CG	TYR	B	693	28.643	62.307	56.567	1.00	0.21	B	C
ATOM	3019	CD1	TYR	B	693	27.384	61.976	57.031	1.00	0.00	B	C
ATOM	3020	CE1	TYR	B	693	26.509	61.257	56.254	1.00	0.00	B	C
ATOM	3021	CD2	TYR	B	693	29.009	61.875	55.301	1.00	0.00	B	C
ATOM	3022	CE2	TYR	B	693	28.142	61.162	54.521	1.00	0.00	B	C
ATOM	3023	CZ	TYR	B	693	26.889	60.859	55.002	1.00	0.00	B	C
ATOM	3024	OH	TYR	B	693	25.995	60.178	54.226	1.00	0.00	B	O
ATOM	3025	C	TYR	B	693	29.128	65.496	58.404	1.00	4.66	B	C
ATOM	3026	O	TYR	B	693	28.159	65.638	59.143	1.00	4.49	B	O
ATOM	3027	N	ILE	B	694	30.313	66.044	58.627	1.00	5.84	B	N
ATOM	3028	CA	ILE	B	694	30.544	66.881	59.786	1.00	7.29	B	C
ATOM	3029	CB	ILE	B	694	31.909	67.561	59.699	1.00	7.96	B	C
ATOM	3030	CG2	ILE	B	694	32.413	67.878	61.093	1.00	7.05	B	C
ATOM	3031	CG1	ILE	B	694	32.893	66.646	58.970	1.00	8.15	B	C
ATOM	3032	CD1	ILE	B	694	34.271	67.251	58.810	1.00	9.53	B	C
ATOM	3033	C	ILE	B	694	29.446	67.944	59.725	1.00	8.08	B	C
ATOM	3034	O	ILE	B	694	28.719	68.163	60.694	1.00	8.70	B	O
ATOM	3035	N	LYS	B	695	29.323	68.584	58.566	1.00	8.39	B	N
ATOM	3036	CA	LYS	B	695	28.304	69.604	58.366	1.00	7.86	B	C
ATOM	3037	CB	LYS	B	695	28.276	70.045	56.894	1.00	8.09	B	C
ATOM	3038	CG	LYS	B	695	27.390	71.261	56.627	1.00	7.39	B	C
ATOM	3039	CD	LYS	B	695	27.419	71.711	55.172	1.00	6.42	B	C
ATOM	3040	CE	LYS	B	695	28.729	72.376	54.794	1.00	5.81	B	C

ATOM	3041	NZ	LYS	B	695	28.593	73.086	53.478	1.00	5.33	B	N
ATOM	3042	C	LYS	B	695	26.936	69.051	58.771	1.00	6.82	B	C
ATOM	3043	O	LYS	B	695	26.113	69.764	59.349	1.00	7.82	B	O
ATOM	3044	N	GLU	B	696	26.701	67.778	58.467	1.00	4.95	B	N
ATOM	3045	CA	GLU	B	696	25.440	67.141	58.803	1.00	4.52	B	C
ATOM	3046	CB	GLU	B	696	25.348	65.764	58.154	1.00	5.55	B	C
ATOM	3047	CG	GLU	B	696	23.935	65.246	58.008	1.00	5.27	B	C
ATOM	3048	CD	GLU	B	696	23.094	66.164	57.143	1.00	5.89	B	C
ATOM	3049	OE1	GLU	B	696	23.575	66.553	56.052	1.00	5.79	B	O
ATOM	3050	OE2	GLU	B	696	21.957	66.493	57.552	1.00	5.89	B	O
ATOM	3051	C	GLU	B	696	25.357	67.006	60.312	1.00	4.52	B	C
ATOM	3052	O	GLU	B	696	24.267	66.951	60.877	1.00	4.75	B	O
ATOM	3053	N	LEU	B	697	26.515	66.927	60.964	1.00	4.74	B	N
ATOM	3054	CA	LEU	B	697	26.560	66.837	62.422	1.00	3.38	B	C
ATOM	3055	CB	LEU	B	697	27.911	66.278	62.896	1.00	2.21	B	C
ATOM	3056	CG	LEU	B	697	28.264	66.292	64.394	1.00	1.22	B	C
ATOM	3057	CD1	LEU	B	697	27.194	65.613	65.199	1.00	0.00	B	C
ATOM	3058	CD2	LEU	B	697	29.589	65.604	64.617	1.00	0.45	B	C
ATOM	3059	C	LEU	B	697	26.380	68.273	62.902	1.00	3.38	B	C
ATOM	3060	O	LEU	B	697	25.852	68.518	63.986	1.00	3.61	B	O
ATOM	3061	N	GLY	B	698	26.822	69.213	62.066	1.00	2.53	B	N
ATOM	3062	CA	GLY	B	698	26.703	70.626	62.370	1.00	4.48	B	C
ATOM	3063	C	GLY	B	698	25.299	71.122	62.057	1.00	4.73	B	C
ATOM	3064	O	GLY	B	698	25.091	72.232	61.548	1.00	4.58	B	O
ATOM	3065	N	LYS	B	699	24.328	70.269	62.355	1.00	3.99	B	N
ATOM	3066	CA	LYS	B	699	22.921	70.569	62.150	1.00	4.96	B	C
ATOM	3067	CB	LYS	B	699	22.481	70.113	60.762	1.00	5.53	B	C
ATOM	3068	CG	LYS	B	699	23.143	70.858	59.621	1.00	4.15	B	C
ATOM	3069	CD	LYS	B	699	22.555	70.434	58.282	1.00	3.04	B	C
ATOM	3070	CE	LYS	B	699	23.091	71.310	57.168	1.00	3.26	B	C
ATOM	3071	NZ	LYS	B	699	22.909	72.756	57.502	1.00	2.13	B	N
ATOM	3072	C	LYS	B	699	22.227	69.752	63.219	1.00	5.61	B	C
ATOM	3073	O	LYS	B	699	21.105	70.032	63.632	1.00	5.25	B	O
ATOM	3074	N	ALA	B	700	22.957	68.739	63.665	1.00	6.56	B	N
ATOM	3075	CA	ALA	B	700	22.521	67.801	64.684	1.00	5.10	B	C
ATOM	3076	CB	ALA	B	700	23.506	66.624	64.743	1.00	5.71	B	C
ATOM	3077	C	ALA	B	700	22.432	68.482	66.042	1.00	3.16	B	C
ATOM	3078	O	ALA	B	700	21.549	68.168	66.845	1.00	3.56	B	O
ATOM	3079	N	ILE	B	701	23.368	69.394	66.293	1.00	0.09	B	N
ATOM	3080	CA	ILE	B	701	23.408	70.142	67.540	1.00	0.00	B	C
ATOM	3081	CB	ILE	B	701	24.775	70.757	67.782	1.00	0.00	B	C
ATOM	3082	CG2	ILE	B	701	24.771	71.501	69.107	1.00	0.00	B	C
ATOM	3083	CG1	ILE	B	701	25.848	69.665	67.736	1.00	0.00	B	C
ATOM	3084	CD1	ILE	B	701	27.263	70.193	67.810	1.00	0.00	B	C
ATOM	3085	C	ILE	B	701	22.412	71.263	67.383	1.00	0.27	B	C
ATOM	3086	O	ILE	B	701	21.834	71.747	68.352	1.00	0.51	B	O
ATOM	3087	N	VAL	B	702	22.236	71.679	66.135	1.00	0.95	B	N
ATOM	3088	CA	VAL	B	702	21.279	72.713	65.802	1.00	0.00	B	C
ATOM	3089	CB	VAL	B	702	21.210	72.924	64.273	1.00	0.00	B	C
ATOM	3090	CG1	VAL	B	702	19.961	73.672	63.895	1.00	0.00	B	C
ATOM	3091	CG2	VAL	B	702	22.429	73.686	63.815	1.00	0.00	B	C
ATOM	3092	C	VAL	B	702	19.967	72.155	66.313	1.00	0.00	B	C
ATOM	3093	O	VAL	B	702	19.546	72.489	67.411	1.00	0.85	B	O
ATOM	3094	N	LYS	B	703	19.366	71.267	65.518	1.00	0.31	B	N
ATOM	3095	CA	LYS	B	703	18.096	70.604	65.823	1.00	1.08	B	C
ATOM	3096	CB	LYS	B	703	18.094	69.201	65.229	1.00	0.26	B	C
ATOM	3097	CG	LYS	B	703	18.257	69.136	63.735	1.00	0.13	B	C
ATOM	3098	CD	LYS	B	703	16.931	69.311	63.033	1.00	0.00	B	C
ATOM	3099	CE	LYS	B	703	15.996	68.144	63.305	1.00	0.00	B	C
ATOM	3100	NZ	LYS	B	703	14.704	68.283	62.569	1.00	1.13	B	N
ATOM	3101	C	LYS	B	703	17.832	70.485	67.315	1.00	2.26	B	C
ATOM	3102	O	LYS	B	703	16.847	71.013	67.842	1.00	2.34	B	O
ATOM	3103	N	ARG	B	704	18.728	69.779	67.990	1.00	2.65	B	N
ATOM	3104	CA	ARG	B	704	18.611	69.547	69.413	1.00	3.64	B	C
ATOM	3105	CB	ARG	B	704	19.887	68.918	69.924	1.00	0.40	B	C
ATOM	3106	CG	ARG	B	704	20.220	67.666	69.178	1.00	1.83	B	C
ATOM	3107	CD	ARG	B	704	19.070	66.659	69.305	1.00	2.99	B	C
ATOM	3108	NE	ARG	B	704	18.300	66.463	68.077	1.00	3.97	B	N
ATOM	3109	CZ	ARG	B	704	17.032	66.071	68.053	1.00	5.49	B	C
ATOM	3110	NH1	ARG	B	704	16.391	65.834	69.188	1.00	5.67	B	N
ATOM	3111	NH2	ARG	B	704	16.409	65.932	66.895	1.00	6.40	B	N
ATOM	3112	C	ARG	B	704	18.303	70.795	70.198	1.00	5.20	B	C
ATOM	3113	O	ARG	B	704	18.081	70.706	71.403	1.00	6.25	B	O
ATOM	3114	N	GLU	B	705	18.300	71.945	69.512	1.00	7.79	B	N
ATOM	3115	CA	GLU	B	705	18.016	73.257	70.097	1.00	10.11	B	C
ATOM	3116	CB	GLU	B	705	18.441	73.292	71.559	1.00	8.13	B	C
ATOM	3117	CG	GLU	B	705	19.905	72.995	71.770	1.00	4.29	B	C
ATOM	3118	CD	GLU	B	705	20.237	72.854	73.220	1.00	2.54	B	C
ATOM	3119	OE1	GLU	B	705	21.444	72.769	73.529	1.00	1.25	B	O
ATOM	3120	OE2	GLU	B	705	19.289	72.821	74.040	1.00	1.18	B	O
ATOM	3121	C	GLU	B	705	18.703	74.415	69.358	1.00	12.33	B	C

ATOM	3122	O	GLU	B	705	18.041	75.154	68.615	1.00	13.95	B	O
ATOM	3123	N	GLY	B	706	20.018	74.573	69.585	1.00	14.16	B	N
ATOM	3124	CA	GLY	B	706	20.818	75.636	68.965	1.00	13.17	B	C
ATOM	3125	C	GLY	B	706	21.857	76.300	69.884	1.00	12.57	B	C
ATOM	3126	O	GLY	B	706	22.468	75.630	70.715	1.00	13.32	B	O
ATOM	3127	N	ASN	B	707	22.061	77.612	69.721	1.00	10.85	B	N
ATOM	3128	CA	ASN	B	707	22.995	78.429	70.522	1.00	9.37	B	C
ATOM	3129	CB	ASN	B	707	22.807	78.163	72.024	1.00	4.43	B	C
ATOM	3130	CG	ASN	B	707	23.283	79.332	72.907	1.00	1.14	B	C
ATOM	3131	OD1	ASN	B	707	23.256	79.231	74.138	1.00	0.00	B	O
ATOM	3132	ND2	ASN	B	707	23.703	80.445	72.285	1.00	0.00	B	N
ATOM	3133	C	ASN	B	707	24.453	78.209	70.168	1.00	10.22	B	C
ATOM	3134	O	ASN	B	707	25.072	77.304	70.704	1.00	9.72	B	O
ATOM	3135	N	SER	B	708	24.999	79.053	69.287	1.00	11.07	B	N
ATOM	3136	CA	SER	B	708	26.402	78.946	68.848	1.00	10.55	B	C
ATOM	3137	CB	SER	B	708	26.818	80.153	68.011	1.00	10.18	B	C
ATOM	3138	OG	SER	B	708	28.167	80.022	67.597	1.00	9.62	B	O
ATOM	3139	C	SER	B	708	27.417	78.766	69.964	1.00	9.98	B	C
ATOM	3140	O	SER	B	708	28.271	77.897	69.871	1.00	11.36	B	O
ATOM	3141	N	SER	B	709	27.351	79.589	71.007	1.00	8.07	B	N
ATOM	3142	CA	SER	B	709	28.280	79.431	72.128	1.00	6.88	B	C
ATOM	3143	CB	SER	B	709	28.008	80.479	73.223	1.00	5.22	B	C
ATOM	3144	OG	SER	B	709	28.387	81.783	72.807	1.00	0.00	B	O
ATOM	3145	C	SER	B	709	28.102	78.006	72.681	1.00	7.90	B	C
ATOM	3146	O	SER	B	709	28.894	77.539	73.494	1.00	7.38	B	O
ATOM	3147	N	GLN	B	710	27.035	77.344	72.231	1.00	9.50	B	N
ATOM	3148	CA	GLN	B	710	26.716	75.960	72.592	1.00	10.39	B	C
ATOM	3149	CB	GLN	B	710	25.340	75.863	73.308	1.00	10.55	B	C
ATOM	3150	CG	GLN	B	710	25.315	76.239	74.818	1.00	10.48	B	C
ATOM	3151	CD	GLN	B	710	24.160	75.571	75.621	1.00	11.08	B	C
ATOM	3152	OE1	GLN	B	710	23.957	75.858	76.811	1.00	10.52	B	O
ATOM	3153	NE2	GLN	B	710	23.416	74.681	74.969	1.00	11.14	B	N
ATOM	3154	C	GLN	B	710	26.715	75.108	71.288	1.00	10.56	B	C
ATOM	3155	O	GLN	B	710	26.650	73.871	71.334	1.00	10.61	B	O
ATOM	3156	N	ASN	B	711	26.789	75.790	70.139	1.00	9.99	B	N
ATOM	3157	CA	ASN	B	711	26.816	75.156	68.811	1.00	9.16	B	C
ATOM	3158	CB	ASN	B	711	26.449	76.162	67.702	1.00	8.67	B	C
ATOM	3159	CG	ASN	B	711	24.950	76.295	67.491	1.00	10.16	B	C
ATOM	3160	OD1	ASN	B	711	24.496	77.064	66.639	1.00	10.33	B	O
ATOM	3161	ND2	ASN	B	711	24.173	75.540	68.260	1.00	9.68	B	N
ATOM	3162	C	ASN	B	711	28.224	74.648	68.535	1.00	8.24	B	C
ATOM	3163	O	ASN	B	711	28.421	73.549	68.002	1.00	9.11	B	O
ATOM	3164	N	TRP	B	712	29.195	75.490	68.869	1.00	6.81	B	N
ATOM	3165	CA	TRP	B	712	30.594	75.169	68.697	1.00	5.94	B	C
ATOM	3166	CB	TRP	B	712	31.303	76.280	67.901	1.00	3.07	B	C
ATOM	3167	CG	TRP	B	712	31.301	76.034	66.393	1.00	3.11	B	C
ATOM	3168	CD2	TRP	B	712	30.732	76.868	65.375	1.00	1.42	B	C
ATOM	3169	CE2	TRP	B	712	30.958	76.227	64.130	1.00	0.18	B	C
ATOM	3170	CE3	TRP	B	712	30.054	78.094	65.391	1.00	2.04	B	C
ATOM	3171	CD1	TRP	B	712	31.835	74.952	65.735	1.00	2.07	B	C
ATOM	3172	NE1	TRP	B	712	31.631	75.063	64.381	1.00	0.40	B	N
ATOM	3173	CZ2	TRP	B	712	30.530	76.767	62.918	1.00	0.00	B	C
ATOM	3174	CZ3	TRP	B	712	29.624	78.638	64.174	1.00	2.40	B	C
ATOM	3175	CH2	TRP	B	712	29.867	77.970	62.955	1.00	1.97	B	C
ATOM	3176	C	TRP	B	712	31.184	74.983	70.095	1.00	6.35	B	C
ATOM	3177	O	TRP	B	712	32.350	75.276	70.346	1.00	5.67	B	O
ATOM	3178	N	GLN	B	713	30.337	74.480	70.996	1.00	7.11	B	N
ATOM	3179	CA	GLN	B	713	30.682	74.192	72.397	1.00	6.46	B	C
ATOM	3180	CB	GLN	B	713	29.889	75.111	73.329	1.00	4.90	B	C
ATOM	3181	CG	GLN	B	713	30.613	75.478	74.624	1.00	4.23	B	C
ATOM	3182	CD	GLN	B	713	30.752	74.322	75.597	1.00	2.92	B	C
ATOM	3183	OE1	GLN	B	713	31.671	74.298	76.421	1.00	0.00	B	O
ATOM	3184	NE2	GLN	B	713	29.827	73.366	75.520	1.00	2.38	B	N
ATOM	3185	C	GLN	B	713	30.338	72.717	72.706	1.00	6.53	B	C
ATOM	3186	O	GLN	B	713	30.963	72.062	73.544	1.00	6.06	B	O
ATOM	3187	N	ARG	B	714	29.323	72.209	72.023	1.00	5.38	B	N
ATOM	3188	CA	ARG	B	714	28.914	70.829	72.191	1.00	5.07	B	C
ATOM	3189	CB	ARG	B	714	27.397	70.688	72.054	1.00	6.07	B	C
ATOM	3190	CG	ARG	B	714	26.896	69.335	72.499	1.00	6.36	B	C
ATOM	3191	CD	ARG	B	714	25.455	69.114	72.131	1.00	5.08	B	C
ATOM	3192	NE	ARG	B	714	25.107	67.711	72.311	1.00	2.45	B	N
ATOM	3193	CZ	ARG	B	714	25.072	67.098	73.487	1.00	2.10	B	C
ATOM	3194	NH1	ARG	B	714	25.356	67.762	74.601	1.00	0.62	B	N
ATOM	3195	NH2	ARG	B	714	24.768	65.814	73.541	1.00	0.41	B	N
ATOM	3196	C	ARG	B	714	29.598	70.095	71.067	1.00	3.98	B	C
ATOM	3197	O	ARG	B	714	30.019	68.956	71.213	1.00	3.65	B	O
ATOM	3198	N	PHE	B	715	29.706	70.759	69.929	1.00	3.76	B	N
ATOM	3199	CA	PHE	B	715	30.384	70.139	68.817	1.00	3.39	B	C
ATOM	3200	CB	PHE	B	715	30.523	71.064	67.630	1.00	1.29	B	C
ATOM	3201	CG	PHE	B	715	31.399	70.505	66.567	1.00	0.25	B	C
ATOM	3202	CD1	PHE	B	715	30.858	69.805	65.513	1.00	0.00	B	C

ATOM	3203	CD2	PHE	B	715	32.780	70.655	66.639	1.00	0.82	B	C
ATOM	3204	CE1	PHE	B	715	31.674	69.261	64.539	1.00	0.03	B	C
ATOM	3205	CE2	PHE	B	715	33.610	70.113	65.669	1.00	0.11	B	C
ATOM	3206	CZ	PHE	B	715	33.053	69.415	64.615	1.00	0.16	B	C
ATOM	3207	C	PHE	B	715	31.761	69.854	69.333	1.00	4.65	B	C
ATOM	3208	O	PHE	B	715	32.459	68.983	68.829	1.00	3.77	B	O
ATOM	3209	N	TYR	B	716	32.182	70.623	70.324	1.00	6.63	B	N
ATOM	3210	CA	TYR	B	716	33.486	70.349	70.872	1.00	7.92	B	C
ATOM	3211	CB	TYR	B	716	33.990	71.465	71.761	1.00	6.92	B	C
ATOM	3212	CG	TYR	B	716	35.299	71.058	72.378	1.00	8.08	B	C
ATOM	3213	CD1	TYR	B	716	35.361	70.563	73.677	1.00	7.50	B	C
ATOM	3214	CE1	TYR	B	716	36.554	70.102	74.211	1.00	7.63	B	C
ATOM	3215	CD2	TYR	B	716	36.469	71.081	71.629	1.00	7.55	B	C
ATOM	3216	CE2	TYR	B	716	37.660	70.621	72.155	1.00	8.05	B	C
ATOM	3217	CZ	TYR	B	716	37.694	70.136	73.444	1.00	8.52	B	C
ATOM	3218	OH	TYR	B	716	38.883	69.710	73.967	1.00	9.86	B	O
ATOM	3219	C	TYR	B	716	33.386	69.075	71.696	1.00	7.95	B	C
ATOM	3220	O	TYR	B	716	34.155	68.132	71.494	1.00	10.20	B	O
ATOM	3221	N	GLN	B	717	32.438	69.047	72.626	1.00	6.46	B	N
ATOM	3222	CA	GLN	B	717	32.243	67.878	73.466	1.00	5.43	B	C
ATOM	3223	CB	GLN	B	717	31.111	68.150	74.438	1.00	6.05	B	C
ATOM	3224	CG	GLN	B	717	31.448	69.250	75.397	1.00	4.00	B	C
ATOM	3225	CD	GLN	B	717	32.885	69.145	75.858	1.00	3.08	B	C
ATOM	3226	OE1	GLN	B	717	33.397	68.044	76.106	1.00	1.83	B	O
ATOM	3227	NE2	GLN	B	717	33.549	70.290	75.976	1.00	3.63	B	N
ATOM	3228	C	GLN	B	717	31.968	66.606	72.662	1.00	5.10	B	C
ATOM	3229	O	GLN	B	717	32.465	65.535	72.998	1.00	5.64	B	O
ATOM	3230	N	LEU	B	718	31.182	66.724	71.598	1.00	4.88	B	N
ATOM	3231	CA	LEU	B	718	30.890	65.570	70.759	1.00	4.55	B	C
ATOM	3232	CB	LEU	B	718	29.726	65.865	69.814	1.00	4.11	B	C
ATOM	3233	CG	LEU	B	718	28.323	65.978	70.424	1.00	3.81	B	C
ATOM	3234	CD1	LEU	B	718	27.312	66.266	69.310	1.00	3.13	B	C
ATOM	3235	CD2	LEU	B	718	27.970	64.693	71.158	1.00	3.26	B	C
ATOM	3236	C	LEU	B	718	32.111	65.134	69.946	1.00	4.69	B	O
ATOM	3237	O	LEU	B	718	32.229	63.975	69.589	1.00	5.53	B	O
ATOM	3238	N	THR	B	719	33.010	66.063	69.634	1.00	4.08	B	N
ATOM	3239	CA	THR	B	719	34.216	65.711	68.887	1.00	2.90	B	C
ATOM	3240	CB	THR	B	719	34.709	66.871	67.986	1.00	2.25	B	C
ATOM	3241	OG1	THR	B	719	33.829	67.000	66.867	1.00	0.00	B	O
ATOM	3242	CG2	THR	B	719	36.118	66.599	67.460	1.00	1.41	B	C
ATOM	3243	C	THR	B	719	35.276	65.340	69.916	1.00	3.68	B	C
ATOM	3244	O	THR	B	719	36.429	65.050	69.583	1.00	3.77	B	O
ATOM	3245	N	LYS	B	720	34.854	65.336	71.177	1.00	3.64	B	N
ATOM	3246	CA	LYS	B	720	35.731	64.969	72.278	1.00	4.68	B	C
ATOM	3247	CB	LYS	B	720	35.302	65.690	73.555	1.00	4.92	B	C
ATOM	3248	CG	LYS	B	720	36.318	65.634	74.661	1.00	4.64	B	C
ATOM	3249	CD	LYS	B	720	37.574	66.396	74.288	1.00	5.28	B	C
ATOM	3250	CE	LYS	B	720	38.617	66.334	75.414	1.00	6.57	B	C
ATOM	3251	NZ	LYS	B	720	38.118	66.864	76.727	1.00	7.22	B	N
ATOM	3252	C	LYS	B	720	35.567	63.455	72.437	1.00	5.20	B	C
ATOM	3253	O	LYS	B	720	36.549	62.711	72.579	1.00	5.84	B	O
ATOM	3254	N	LEU	B	721	34.312	63.010	72.401	1.00	5.57	B	N
ATOM	3255	CA	LEU	B	721	34.005	61.593	72.511	1.00	5.98	B	C
ATOM	3256	CB	LEU	B	721	32.514	61.352	72.317	1.00	5.57	B	C
ATOM	3257	CG	LEU	B	721	32.079	59.897	72.465	1.00	6.62	B	C
ATOM	3258	CD1	LEU	B	721	32.392	59.429	73.874	1.00	6.68	B	C
ATOM	3259	CD2	LEU	B	721	30.603	59.755	72.188	1.00	5.90	B	C
ATOM	3260	C	LEU	B	721	34.770	60.890	71.405	1.00	5.67	B	O
ATOM	3261	O	LEU	B	721	35.740	60.193	71.660	1.00	5.59	B	O
ATOM	3262	N	LEU	B	722	34.330	61.090	70.169	1.00	4.94	B	N
ATOM	3263	CA	LEU	B	722	34.983	60.485	69.015	1.00	2.16	B	C
ATOM	3264	CB	LEU	B	722	34.472	61.102	67.712	1.00	1.76	B	C
ATOM	3265	CG	LEU	B	722	33.008	60.891	67.372	1.00	0.00	B	C
ATOM	3266	CD1	LEU	B	722	32.697	61.525	66.045	1.00	0.00	B	C
ATOM	3267	CD2	LEU	B	722	32.733	59.419	67.326	1.00	0.00	B	C
ATOM	3268	C	LEU	B	722	36.479	60.676	69.087	1.00	0.69	B	C
ATOM	3269	O	LEU	B	722	37.231	60.049	68.354	1.00	2.70	B	O
ATOM	3270	N	ASP	B	723	36.917	61.568	69.956	1.00	0.00	B	N
ATOM	3271	CA	ASP	B	723	38.339	61.795	70.086	1.00	0.13	B	C
ATOM	3272	CB	ASP	B	723	38.599	63.220	70.569	1.00	3.91	B	C
ATOM	3273	CG	ASP	B	723	39.140	64.107	69.475	1.00	3.14	B	C
ATOM	3274	OD1	ASP	B	723	38.599	64.029	68.350	1.00	4.00	B	O
ATOM	3275	OD2	ASP	B	723	40.096	64.875	69.744	1.00	4.32	B	O
ATOM	3276	C	ASP	B	723	38.929	60.781	71.050	1.00	0.90	B	C
ATOM	3277	O	ASP	B	723	40.086	60.377	70.907	1.00	0.00	B	O
ATOM	3278	N	SER	B	724	38.119	60.373	72.027	1.00	0.71	B	N
ATOM	3279	CA	SER	B	724	38.528	59.388	73.023	1.00	0.56	B	C
ATOM	3280	CB	SER	B	724	37.854	59.702	74.361	1.00	0.00	B	C
ATOM	3281	OG	SER	B	724	36.451	59.702	74.232	1.00	0.00	B	O
ATOM	3282	C	SER	B	724	38.211	57.944	72.583	1.00	0.12	B	C
ATOM	3283	O	SER	B	724	38.191	57.032	73.402	1.00	0.00	B	O

ATOM	3284	N	MET	B	725	38.003	57.763	71.278	1.00	0.88	B	N
ATOM	3285	CA	MET	B	725	37.677	56.477	70.651	1.00	2.25	B	C
ATOM	3286	CB	MET	B	725	36.884	56.723	69.365	1.00	1.01	B	C
ATOM	3287	CG	MET	B	725	35.673	55.837	69.188	1.00	0.00	B	C
ATOM	3288	SD	MET	B	725	34.481	56.042	70.509	1.00	0.00	B	S
ATOM	3289	CE	MET	B	725	34.683	54.584	71.419	1.00	0.00	B	C
ATOM	3290	C	MET	B	725	38.907	55.632	70.311	1.00	3.98	B	C
ATOM	3291	O	MET	B	725	39.003	54.462	70.705	1.00	4.97	B	O
ATOM	3292	N	HIS	B	726	39.835	56.218	69.559	1.00	5.71	B	N
ATOM	3293	CA	HIS	B	726	41.058	55.517	69.167	1.00	6.96	B	C
ATOM	3294	CB	HIS	B	726	42.006	56.457	68.413	1.00	8.10	B	C
ATOM	3295	CG	HIS	B	726	41.413	57.074	67.183	1.00	8.94	B	C
ATOM	3296	CD2	HIS	B	726	41.818	57.045	65.891	1.00	9.06	B	C
ATOM	3297	ND1	HIS	B	726	40.305	57.893	67.219	1.00	9.43	B	N
ATOM	3298	CE1	HIS	B	726	40.057	58.347	66.002	1.00	9.27	B	C
ATOM	3299	NE2	HIS	B	726	40.961	57.847	65.179	1.00	9.37	B	N
ATOM	3300	C	HIS	B	726	41.806	54.931	70.375	1.00	7.08	B	C
ATOM	3301	O	HIS	B	726	42.576	53.981	70.239	1.00	7.67	B	O
ATOM	3302	N	GLU	B	727	41.596	55.505	71.552	1.00	6.44	B	N
ATOM	3303	CA	GLU	B	727	42.271	55.007	72.735	1.00	5.32	B	C
ATOM	3304	CB	GLU	B	727	42.583	56.164	73.702	1.00	6.18	B	C
ATOM	3305	CG	GLU	B	727	43.413	57.299	73.079	1.00	8.03	B	C
ATOM	3306	CD	GLU	B	727	44.439	57.919	74.040	1.00	7.60	B	C
ATOM	3307	OE1	GLU	B	727	44.041	58.371	75.136	1.00	8.03	B	O
ATOM	3308	OE2	GLU	B	727	45.645	57.955	73.686	1.00	7.05	B	O
ATOM	3309	C	GLU	B	727	41.436	53.939	73.432	1.00	3.62	B	C
ATOM	3310	O	GLU	B	727	41.808	53.434	74.486	1.00	3.55	B	O
ATOM	3311	N	VAL	B	728	40.298	53.596	72.846	1.00	2.22	B	N
ATOM	3312	CA	VAL	B	728	39.444	52.569	73.433	1.00	0.71	B	C
ATOM	3313	CB	VAL	B	728	37.954	52.913	73.303	1.00	0.06	B	C
ATOM	3314	CG1	VAL	B	728	37.117	51.715	73.658	1.00	0.00	B	C
ATOM	3315	CG2	VAL	B	728	37.612	54.063	74.230	1.00	0.00	B	C
ATOM	3316	C	VAL	B	728	39.715	51.290	72.682	1.00	1.27	B	C
ATOM	3317	O	VAL	B	728	40.245	50.335	73.237	1.00	0.00	B	O
ATOM	3318	N	VAL	B	729	39.359	51.303	71.403	1.00	1.98	B	N
ATOM	3319	CA	VAL	B	729	39.558	50.176	70.501	1.00	2.75	B	C
ATOM	3320	CB	VAL	B	729	39.342	50.624	69.047	1.00	3.17	B	C
ATOM	3321	CG1	VAL	B	729	39.385	49.446	68.120	1.00	2.91	B	C
ATOM	3322	CG2	VAL	B	729	38.019	51.345	68.934	1.00	4.71	B	C
ATOM	3323	C	VAL	B	729	40.936	49.513	70.633	1.00	1.91	B	C
ATOM	3324	O	VAL	B	729	41.043	48.314	70.399	1.00	2.81	B	O
ATOM	3325	N	GLU	B	730	41.979	50.273	70.994	1.00	0.64	B	N
ATOM	3326	CA	GLU	B	730	43.312	49.687	71.182	1.00	0.00	B	C
ATOM	3327	CB	GLU	B	730	44.388	50.730	71.535	1.00	0.30	B	C
ATOM	3328	CG	GLU	B	730	45.844	50.139	71.573	1.00	0.29	B	C
ATOM	3329	CD	GLU	B	730	46.697	50.534	72.812	1.00	1.21	B	C
ATOM	3330	OE1	GLU	B	730	47.872	50.095	72.884	1.00	0.14	B	O
ATOM	3331	OE2	GLU	B	730	46.211	51.266	73.708	1.00	1.95	B	O
ATOM	3332	C	GLU	B	730	43.159	48.774	72.371	1.00	0.00	B	C
ATOM	3333	O	GLU	B	730	43.607	47.629	72.358	1.00	0.00	B	O
ATOM	3334	N	ASN	B	731	42.524	49.305	73.409	1.00	0.00	B	N
ATOM	3335	CA	ASN	B	731	42.291	48.524	74.606	1.00	0.00	B	C
ATOM	3336	CB	ASN	B	731	41.718	49.409	75.712	1.00	0.00	B	C
ATOM	3337	CG	ASN	B	731	42.754	50.309	76.310	1.00	0.00	B	C
ATOM	3338	OD1	ASN	B	731	42.729	50.604	77.501	1.00	0.00	B	O
ATOM	3339	ND2	ASN	B	731	43.678	50.756	75.485	1.00	0.00	B	N
ATOM	3340	C	ASN	B	731	41.376	47.318	74.341	1.00	0.52	B	C
ATOM	3341	O	ASN	B	731	41.568	46.239	74.901	1.00	0.39	B	O
ATOM	3342	N	LEU	B	732	40.382	47.488	73.486	1.00	1.09	B	N
ATOM	3343	CA	LEU	B	732	39.511	46.376	73.196	1.00	0.92	B	C
ATOM	3344	CB	LEU	B	732	38.152	46.865	72.714	1.00	0.49	B	C
ATOM	3345	CG	LEU	B	732	37.438	47.757	73.733	1.00	0.20	B	C
ATOM	3346	CD1	LEU	B	732	36.011	47.964	73.293	1.00	0.28	B	C
ATOM	3347	CD2	LEU	B	732	37.464	47.132	75.106	1.00	0.00	B	C
ATOM	3348	C	LEU	B	732	40.185	45.510	72.155	1.00	1.11	B	C
ATOM	3349	O	LEU	B	732	40.225	44.291	72.305	1.00	3.42	B	O
ATOM	3350	N	LEU	B	733	40.725	46.111	71.099	1.00	1.44	B	N
ATOM	3351	CA	LEU	B	733	41.418	45.291	70.111	1.00	2.90	B	C
ATOM	3352	CB	LEU	B	733	42.073	46.156	69.034	1.00	2.85	B	C
ATOM	3353	CG	LEU	B	733	41.055	46.857	68.125	1.00	5.50	B	C
ATOM	3354	CD1	LEU	B	733	41.775	47.732	67.080	1.00	4.61	B	C
ATOM	3355	CD2	LEU	B	733	40.174	45.810	67.450	1.00	5.90	B	C
ATOM	3356	C	LEU	B	733	42.476	44.476	70.862	1.00	3.78	B	C
ATOM	3357	O	LEU	B	733	42.646	43.274	70.643	1.00	0.14	B	O
ATOM	3358	N	ASN	B	734	43.174	45.137	71.773	1.00	5.04	B	N
ATOM	3359	CA	ASN	B	734	44.176	44.450	72.550	1.00	4.70	B	C
ATOM	3360	CB	ASN	B	734	45.066	45.449	73.283	1.00	2.89	B	C
ATOM	3361	CG	ASN	B	734	46.040	46.120	72.353	1.00	2.49	B	C
ATOM	3362	OD1	ASN	B	734	45.656	46.611	71.295	1.00	2.65	B	O
ATOM	3363	ND2	ASN	B	734	47.311	46.133	72.731	1.00	2.94	B	N
ATOM	3364	C	ASN	B	734	43.465	43.543	73.514	1.00	4.82	B	C

ATOM	3365	O	ASN B 734	43.767	43.521	74.701	1.00	4.52	B	O
ATOM	3366	N	TYR B 735	42.491	42.814	72.986	1.00	5.58	B	N
ATOM	3367	CA	TYR B 735	41.721	41.840	73.756	1.00	6.62	B	C
ATOM	3368	CB	TYR B 735	40.949	42.525	74.891	1.00	6.55	B	C
ATOM	3369	CG	TYR B 735	41.185	41.886	76.248	1.00	7.79	B	C
ATOM	3370	CD1	TYR B 735	40.832	40.548	76.485	1.00	6.95	B	C
ATOM	3371	CE1	TYR B 735	41.076	39.944	77.719	1.00	5.60	B	C
ATOM	3372	CD2	TYR B 735	41.787	42.607	77.287	1.00	5.97	B	C
ATOM	3373	CE2	TYR B 735	42.039	42.016	78.522	1.00	4.72	B	C
ATOM	3374	CZ	TYR B 735	41.686	40.682	78.732	1.00	5.67	B	C
ATOM	3375	OH	TYR B 735	41.976	40.083	79.942	1.00	5.49	B	O
ATOM	3376	C	TYR B 735	40.769	41.059	72.836	1.00	7.21	B	C
ATOM	3377	O	TYR B 735	40.257	40.005	73.210	1.00	6.05	B	O
ATOM	3378	N	CYS B 736	40.547	41.575	71.628	1.00	7.12	B	N
ATOM	3379	CA	CYS B 736	39.683	40.915	70.655	1.00	6.77	B	C
ATOM	3380	CB	CYS B 736	38.601	41.873	70.196	1.00	4.98	B	C
ATOM	3381	SG	CYS B 736	39.261	43.200	69.229	1.00	4.31	B	S
ATOM	3382	C	CYS B 736	40.574	40.526	69.483	1.00	7.14	B	C
ATOM	3383	O	CYS B 736	40.126	40.073	68.435	1.00	7.22	B	O
ATOM	3384	N	PHE B 737	41.859	40.741	69.706	1.00	7.85	B	N
ATOM	3385	CA	PHE B 737	42.953	40.445	68.787	1.00	7.06	B	C
ATOM	3386	CB	PHE B 737	43.772	41.726	68.581	1.00	6.71	B	C
ATOM	3387	CG	PHE B 737	45.197	41.494	68.198	1.00	5.22	B	C
ATOM	3388	CD1	PHE B 737	45.576	41.456	66.861	1.00	5.46	B	C
ATOM	3389	CD2	PHE B 737	46.172	41.345	69.177	1.00	5.74	B	C
ATOM	3390	CE1	PHE B 737	46.915	41.272	66.502	1.00	5.11	B	C
ATOM	3391	CE2	PHE B 737	47.520	41.160	68.833	1.00	5.57	B	C
ATOM	3392	CZ	PHE B 737	47.889	41.126	67.495	1.00	4.69	B	C
ATOM	3393	C	PHE B 737	43.738	39.437	69.615	1.00	6.54	B	C
ATOM	3394	O	PHE B 737	44.123	38.379	69.145	1.00	4.30	B	O
ATOM	3395	N	GLN B 738	43.923	39.827	70.874	1.00	6.10	B	N
ATOM	3396	CA	GLN B 738	44.607	39.086	71.916	1.00	6.06	B	C
ATOM	3397	CB	GLN B 738	45.363	40.059	72.822	1.00	5.78	B	C
ATOM	3398	CG	GLN B 738	46.096	39.423	74.008	1.00	8.34	B	C
ATOM	3399	CD	GLN B 738	46.571	40.447	75.050	1.00	9.38	B	C
ATOM	3400	OE1	GLN B 738	47.067	41.529	74.697	1.00	9.00	B	O
ATOM	3401	NE2	GLN B 738	46.434	40.100	76.338	1.00	8.95	B	N
ATOM	3402	C	GLN B 738	43.548	38.363	72.730	1.00	6.13	B	C
ATOM	3403	O	GLN B 738	9999.0009999.0009999.000	1.00	0.00	1.00	0.00	B	O
ATOM	3404	OXT	GLN B 738	9999.0009999.0009999.000	1.00	0.00	1.00	0.00	B	O

END

## GR 2

REMARK coordinates from minimization and B-factor refinement  
 REMARK refinement resolution: 500.0 - 2.8 Å  
 REMARK starting r= 0.3063 free\_r= 0.3305  
 REMARK final r= 0.2662 free\_r= 0.3228  
 REMARK rmsd bonds= 0.011662 rmsd angles= 1.28574  
 REMARK B rmsd for bonded mainchain atoms= 1.444 target= 1.5  
 REMARK B rmsd for bonded sidechain atoms= 1.849 target= 2.0  
 REMARK B rmsd for angle mainchain atoms= 2.513 target= 2.0  
 REMARK B rmsd for angle sidechain atoms= 2.838 target= 2.5  
 REMARK target= mlf final wa= 6.4425  
 REMARK final rweight= 0.1160 (with wa= 6.4425)  
 REMARK md-method= torsion annealing schedule= slowcool  
 REMARK starting temperature= 2000 total md steps= 20 \* 6  
 REMARK cycles= 2 coordinate steps= 20 B-factor steps= 10  
 REMARK sg= P6(5) a= 132.09 b= 132.09 c= 53.048 alpha= 90 beta= 90 gamma= 120  
 REMARK topology file 1 : MSI\_CNX\_TOPPAR:protein.top  
 REMARK topology file 2 : MSI\_CNX\_TOPPAR:dna-rna.top  
 REMARK topology file 3 : MSI\_CNX\_TOPPAR:water.top  
 REMARK topology file 4 : MSI\_CNX\_TOPPAR:ion.top  
 REMARK topology file 5 : 486.top  
 REMARK parameter file 1 : MSI\_CNX\_TOPPAR:protein\_rep.param  
 REMARK parameter file 2 : MSI\_CNX\_TOPPAR:dna-rna\_rep.param  
 REMARK parameter file 3 : MSI\_CNX\_TOPPAR:water\_rep.param  
 REMARK parameter file 4 : MSI\_CNX\_TOPPAR:ion.param  
 REMARK parameter file 5 : 486.par  
 REMARK molecular structure file: gen4-in.mtf  
 REMARK input coordinates: gen4-in.pdb  
 REMARK reflection file= gr2.hkl  
 REMARK ncs= none  
 REMARK B-correction resolution: 6.0 - 2.8  
 REMARK initial B-factor correction applied to fobs :  
 REMARK B11= -6.869 B22= -6.869 B33= 13.738  
 REMARK B12= -11.858 B13= 0.000 B23= 0.000  
 REMARK B-factor correction applied to coordinate array B: -1.363  
 REMARK bulk solvent: (Mask) density level= 0.332998 e/Å<sup>3</sup>, B-factor= 39.2984 Å<sup>2</sup>

REMARK reflections with |Fobs|/sigma\_F < 0.0 rejected  
 REMARK reflections with |Fobs| > 10000 \* rms(Fobs) rejected  
 REMARK theoretical total number of refl. in resol. range: 13246 ( 100.0 % )  
 REMARK number of unobserved reflections (no entry or |F|=0): 94 ( 0.7 % )  
 REMARK number of reflections rejected: 0 ( 0.0 % )  
 REMARK total number of reflections used: 13152 ( 99.3 % )  
 REMARK number of reflections in working set: 12496 ( 94.3 % )  
 REMARK number of reflections in test set: 656 ( 5.0 % )  
 CRYST1 132.090 132.090 53.048 90.00 90.00 120.00 P 65  
 REMARK FILENAME="ref4a.pdb"  
 REMARK DATE:Oct-03-2001 16:22:37 created by user: kauppi  
 REMARK Written by CNX VERSION:2000.12

ATOM	1	CB	THR	A	531	-2.670	61.555	-5.859	1.00	50.89	C
ATOM	2	OG1	THR	A	531	-3.135	62.679	-5.103	1.00	48.57	O
ATOM	3	CG2	THR	A	531	-1.762	60.711	-4.975	1.00	48.62	C
ATOM	4	C	THR	A	531	-0.814	61.045	-7.477	1.00	52.79	C
ATOM	5	O	THR	A	531	-1.062	60.037	-8.143	1.00	55.02	O
ATOM	6	N	THR	A	531	-2.841	62.263	-8.281	1.00	50.10	N
ATOM	7	CA	THR	A	531	-1.911	62.050	-7.128	1.00	51.78	C
ATOM	8	N	LEU	A	532	0.401	61.320	-7.020	1.00	52.00	N
ATOM	9	CA	LEU	A	532	1.523	60.441	-7.303	1.00	51.08	C
ATOM	10	CB	LEU	A	532	2.824	61.218	-7.116	1.00	50.51	C
ATOM	11	CG	LEU	A	532	4.072	60.703	-7.841	1.00	51.65	C
ATOM	12	CD1	LEU	A	532	3.802	60.502	-9.347	1.00	48.90	C
ATOM	13	CD2	LEU	A	532	5.202	61.699	-7.580	1.00	49.14	C
ATOM	14	C	LEU	A	532	1.464	59.196	-6.409	1.00	51.38	C
ATOM	15	O	LEU	A	532	1.784	58.083	-6.838	1.00	52.09	O
ATOM	16	N	VAL	A	533	1.024	59.389	-5.170	1.00	50.11	N
ATOM	17	CA	VAL	A	533	0.897	58.290	-4.219	1.00	47.70	C
ATOM	18	CB	VAL	A	533	0.455	58.798	-2.832	1.00	45.94	C
ATOM	19	CG1	VAL	A	533	1.203	58.058	-1.730	1.00	44.34	C
ATOM	20	CG2	VAL	A	533	0.654	60.292	-2.747	1.00	47.26	C
ATOM	21	C	VAL	A	533	-0.163	57.300	-4.710	1.00	47.79	C
ATOM	22	O	VAL	A	533	0.071	56.097	-4.698	1.00	48.19	O
ATOM	23	N	SER	A	534	-1.323	57.812	-5.128	1.00	47.16	N
ATOM	24	CA	SER	A	534	-2.419	56.977	-5.609	1.00	45.62	C
ATOM	25	CB	SER	A	534	-3.580	57.841	-6.103	1.00	46.31	C
ATOM	26	OG	SER	A	534	-3.350	58.280	-7.433	1.00	45.25	O
ATOM	27	C	SER	A	534	-1.884	56.148	-6.757	1.00	45.18	C
ATOM	28	O	SER	A	534	-2.241	54.983	-6.934	1.00	45.92	O
ATOM	29	N	LEU	A	535	-1.015	56.762	-7.543	1.00	44.07	N
ATOM	30	CA	LEU	A	535	-0.408	56.066	-8.670	1.00	44.62	C
ATOM	31	CB	LEU	A	535	0.400	57.066	-9.502	1.00	42.86	C
ATOM	32	CG	LEU	A	535	0.262	56.968	-11.012	1.00	42.52	C
ATOM	33	CD1	LEU	A	535	0.815	58.251	-11.607	1.00	46.18	C
ATOM	34	CD2	LEU	A	535	0.974	55.732	-11.553	1.00	42.44	C
ATOM	35	C	LEU	A	535	0.489	54.902	-8.177	1.00	44.09	C
ATOM	36	O	LEU	A	535	0.522	53.816	-8.782	1.00	41.93	O
ATOM	37	N	LEU	A	536	1.195	55.150	-7.071	1.00	43.42	N
ATOM	38	CA	LEU	A	536	2.067	54.169	-6.438	1.00	44.57	C
ATOM	39	CB	LEU	A	536	2.945	54.830	-5.359	1.00	44.84	C
ATOM	40	CG	LEU	A	536	4.039	55.792	-5.855	1.00	45.68	C
ATOM	41	CD1	LEU	A	536	4.713	56.427	-4.629	1.00	43.24	C
ATOM	42	CD2	LEU	A	536	5.057	55.058	-6.774	1.00	44.85	C
ATOM	43	C	LEU	A	536	1.244	53.053	-5.802	1.00	45.17	C
ATOM	44	O	LEU	A	536	1.675	51.901	-5.781	1.00	47.88	O
ATOM	45	N	GLU	A	537	0.059	53.393	-5.293	1.00	44.85	N
ATOM	46	CA	GLU	A	537	-0.832	52.410	-4.665	1.00	44.61	C
ATOM	47	CB	GLU	A	537	-2.013	53.111	-3.994	1.00	47.17	C
ATOM	48	CG	GLU	A	537	-1.594	54.116	-2.950	1.00	54.20	C
ATOM	49	CD	GLU	A	537	-2.763	54.781	-2.280	1.00	58.42	C
ATOM	50	OE1	GLU	A	537	-3.023	55.989	-2.551	1.00	61.96	O
ATOM	51	OE2	GLU	A	537	-3.418	54.078	-1.479	1.00	58.56	O
ATOM	52	C	GLU	A	537	-1.361	51.381	-5.655	1.00	42.65	C
ATOM	53	O	GLU	A	537	-1.481	50.207	-5.316	1.00	40.36	O
ATOM	54	N	VAL	A	538	-1.675	51.823	-6.872	1.00	40.84	N
ATOM	55	CA	VAL	A	538	-2.189	50.911	-7.886	1.00	41.93	C
ATOM	56	CB	VAL	A	538	-2.919	51.661	-9.040	1.00	40.65	C
ATOM	57	CG1	VAL	A	538	-4.115	52.374	-8.498	1.00	39.71	C
ATOM	58	CG2	VAL	A	538	-2.006	52.664	-9.691	1.00	42.54	C
ATOM	59	C	VAL	A	538	-1.111	50.036	-8.518	1.00	42.28	C
ATOM	60	O	VAL	A	538	-1.370	48.904	-8.934	1.00	44.13	O
ATOM	61	N	ILE	A	539	0.107	50.544	-8.584	1.00	39.49	N
ATOM	62	CA	ILE	A	539	1.148	49.759	-9.201	1.00	37.83	C
ATOM	63	CB	ILE	A	539	2.220	50.654	-9.818	1.00	38.75	C
ATOM	64	CG2	ILE	A	539	1.572	51.621	-10.827	1.00	33.81	C
ATOM	65	CG1	ILE	A	539	2.997	51.350	-8.705	1.00	35.42	C
ATOM	66	CD1	ILE	A	539	4.177	52.018	-9.234	1.00	28.59	C
ATOM	67	C	ILE	A	539	1.803	48.792	-8.226	1.00	39.36	C
ATOM	68	O	ILE	A	539	2.521	47.867	-8.637	1.00	37.52	O
ATOM	69	N	GLU	A	540	1.540	49.018	-6.939	1.00	39.11	N

ATOM	70	CA	GLU A 540	2.066	48.186	-5.859	1.00	41.15	C
ATOM	71	CB	GLU A 540	1.556	48.676	-4.497	1.00	42.05	C
ATOM	72	CG	GLU A 540	2.064	47.818	-3.332	1.00	45.41	C
ATOM	73	CD	GLU A 540	3.593	47.897	-3.078	1.00	49.27	C
ATOM	74	OE1	GLU A 540	4.101	47.055	-2.298	1.00	50.37	O
ATOM	75	OE2	GLU A 540	4.293	48.782	-3.627	1.00	50.34	O
ATOM	76	C	GLU A 540	1.671	46.736	-6.065	1.00	42.28	C
ATOM	77	O	GLU A 540	0.508	46.355	-5.893	1.00	44.55	O
ATOM	78	N	PRO A 541	2.631	45.884	-6.429	1.00	43.64	N
ATOM	79	CD	PRO A 541	4.082	46.106	-6.517	1.00	41.58	C
ATOM	80	CA	PRO A 541	2.305	44.466	-6.650	1.00	44.10	C
ATOM	81	CB	PRO A 541	3.687	43.826	-6.827	1.00	42.99	C
ATOM	82	CG	PRO A 541	4.519	44.923	-7.348	1.00	42.55	C
ATOM	83	C	PRO A 541	1.498	43.806	-5.505	1.00	45.90	C
ATOM	84	O	PRO A 541	1.446	44.305	-4.383	1.00	46.36	O
ATOM	85	N	GLU A 542	0.867	42.681	-5.796	1.00	47.77	N
ATOM	86	CA	GLU A 542	0.102	41.973	-4.783	1.00	48.76	C
ATOM	87	CB	GLU A 542	-1.141	41.360	-5.423	1.00	51.52	C
ATOM	88	CG	GLU A 542	-1.832	42.255	-6.442	1.00	55.93	C
ATOM	89	CD	GLU A 542	-3.232	41.758	-6.809	1.00	58.75	C
ATOM	90	OE1	GLU A 542	-3.408	40.558	-7.137	1.00	59.24	O
ATOM	91	OE2	GLU A 542	-4.166	42.584	-6.774	1.00	61.55	O
ATOM	92	C	GLU A 542	0.957	40.851	-4.168	1.00	48.92	C
ATOM	93	O	GLU A 542	1.685	40.163	-4.883	1.00	48.86	O
ATOM	94	N	VAL A 543	0.862	40.671	-2.854	1.00	48.50	N
ATOM	95	CA	VAL A 543	1.602	39.635	-2.154	1.00	49.92	C
ATOM	96	CB	VAL A 543	1.045	39.436	-0.722	1.00	50.72	C
ATOM	97	CG1	VAL A 543	1.256	40.707	0.049	1.00	52.12	C
ATOM	98	CG2	VAL A 543	-0.469	39.114	-0.753	1.00	53.53	C
ATOM	99	C	VAL A 543	1.543	38.304	-2.901	1.00	50.83	C
ATOM	100	O	VAL A 543	0.467	37.826	-3.245	1.00	52.03	O
ATOM	101	N	LEU A 544	2.705	37.711	-3.145	1.00	50.91	N
ATOM	102	CA	LEU A 544	2.795	36.458	-3.858	1.00	50.75	C
ATOM	103	CB	LEU A 544	4.063	36.430	-4.702	1.00	49.89	C
ATOM	104	CG	LEU A 544	4.221	37.508	-5.778	1.00	49.94	C
ATOM	105	CD1	LEU A 544	5.440	37.164	-6.652	1.00	45.63	C
ATOM	106	CD2	LEU A 544	2.937	37.613	-6.619	1.00	49.14	C
ATOM	107	C	LEU A 544	2.818	35.301	-2.883	1.00	53.02	C
ATOM	108	O	LEU A 544	3.450	35.385	-1.826	1.00	54.39	O
ATOM	109	N	TYR A 545	2.142	34.215	-3.250	1.00	53.91	N
ATOM	110	CA	TYR A 545	2.069	33.021	-2.415	1.00	54.02	C
ATOM	111	CB	TYR A 545	0.803	32.229	-2.750	1.00	53.76	C
ATOM	112	CG	TYR A 545	-0.439	32.804	-2.126	1.00	54.26	C
ATOM	113	CD1	TYR A 545	-0.790	32.490	-0.814	1.00	53.46	C
ATOM	114	CE1	TYR A 545	-1.912	33.057	-0.215	1.00	55.56	C
ATOM	115	CD2	TYR A 545	-1.240	33.702	-2.831	1.00	55.14	C
ATOM	116	CE2	TYR A 545	-2.363	34.279	-2.246	1.00	56.32	C
ATOM	117	CZ	TYR A 545	-2.695	33.954	-0.938	1.00	57.22	C
ATOM	118	OH	TYR A 545	-3.812	34.526	-0.360	1.00	59.17	O
ATOM	119	C	TYR A 545	3.281	32.143	-2.623	1.00	54.55	C
ATOM	120	O	TYR A 545	3.736	31.983	-3.752	1.00	54.35	O
ATOM	121	N	ALA A 546	3.798	31.571	-1.536	1.00	55.09	N
ATOM	122	CA	ALA A 546	4.968	30.686	-1.602	1.00	56.29	C
ATOM	123	CB	ALA A 546	5.717	30.711	-0.278	1.00	57.16	C
ATOM	124	C	ALA A 546	4.605	29.243	-1.949	1.00	56.88	C
ATOM	125	O	ALA A 546	5.394	28.529	-2.572	1.00	56.57	O
ATOM	126	N	GLY A 547	3.413	28.819	-1.543	1.00	58.20	N
ATOM	127	CA	GLY A 547	2.986	27.461	-1.813	1.00	59.76	C
ATOM	128	C	GLY A 547	3.830	26.466	-1.042	1.00	61.86	C
ATOM	129	O	GLY A 547	4.280	25.465	-1.595	1.00	62.10	O
ATOM	130	N	TYR A 548	4.048	26.743	0.241	1.00	63.15	N
ATOM	131	CA	TYR A 548	4.847	25.868	1.092	1.00	63.46	C
ATOM	132	CB	TYR A 548	5.336	26.648	2.315	1.00	60.97	C
ATOM	133	CG	TYR A 548	6.218	25.845	3.239	1.00	58.20	C
ATOM	134	CD1	TYR A 548	5.862	25.625	4.575	1.00	57.08	C
ATOM	135	CE1	TYR A 548	6.706	24.908	5.442	1.00	54.85	C
ATOM	136	CD2	TYR A 548	7.423	25.332	2.790	1.00	56.61	C
ATOM	137	CE2	TYR A 548	8.265	24.621	3.634	1.00	55.45	C
ATOM	138	CZ	TYR A 548	7.911	24.414	4.957	1.00	54.67	C
ATOM	139	OH	TYR A 548	8.786	23.730	5.777	1.00	53.04	O
ATOM	140	C	TYR A 548	4.029	24.652	1.532	1.00	65.38	C
ATOM	141	O	TYR A 548	2.802	24.666	1.462	1.00	64.30	O
ATOM	142	N	ASP A 549	4.727	23.603	1.964	1.00	68.63	N
ATOM	143	CA	ASP A 549	4.113	22.364	2.438	1.00	70.64	C
ATOM	144	CB	ASP A 549	5.099	21.196	2.236	1.00	70.58	C
ATOM	145	CG	ASP A 549	6.509	21.490	2.777	1.00	69.34	C
ATOM	146	OD1	ASP A 549	6.768	21.277	3.991	1.00	67.80	O
ATOM	147	OD2	ASP A 549	7.365	21.929	1.976	1.00	68.83	O
ATOM	148	C	ASP A 549	3.763	22.563	3.917	1.00	72.67	C
ATOM	149	O	ASP A 549	4.545	22.229	4.812	1.00	73.29	O
ATOM	150	N	SER A 550	2.574	23.116	4.150	1.00	74.78	N

ATOM	151	CA	SER	A	550	2.098	23.447	5.491	1.00	76.11	C
ATOM	152	CB	SER	A	550	0.726	24.099	5.419	1.00	75.82	C
ATOM	153	OG	SER	A	550	-0.274	23.132	5.690	1.00	76.81	O
ATOM	154	C	SER	A	550	2.026	22.331	6.515	1.00	77.29	C
ATOM	155	O	SER	A	550	2.217	22.586	7.699	1.00	78.08	O
ATOM	156	N	SER	A	551	1.716	21.111	6.091	1.00	78.62	N
ATOM	157	CA	SER	A	551	1.637	20.003	7.046	1.00	79.57	C
ATOM	158	CB	SER	A	551	0.564	18.999	6.632	1.00	79.28	C
ATOM	159	OG	SER	A	551	0.966	18.319	5.457	1.00	78.65	O
ATOM	160	C	SER	A	551	2.970	19.279	7.107	1.00	79.32	C
ATOM	161	O	SER	A	551	3.457	18.926	8.184	1.00	80.11	O
ATOM	162	N	VAL	A	552	3.542	19.050	5.931	1.00	78.23	N
ATOM	163	CA	VAL	A	552	4.813	18.362	5.811	1.00	77.87	C
ATOM	164	CB	VAL	A	552	5.374	18.483	4.392	1.00	76.92	C
ATOM	165	CG1	VAL	A	552	6.625	17.630	4.262	1.00	75.03	C
ATOM	166	CG2	VAL	A	552	4.307	18.080	3.375	1.00	76.24	C
ATOM	167	C	VAL	A	552	5.816	18.945	6.783	1.00	78.01	C
ATOM	168	O	VAL	A	552	5.957	20.166	6.899	1.00	78.05	O
ATOM	169	N	PRO	A	553	6.529	18.071	7.502	1.00	78.43	N
ATOM	170	CD	PRO	A	553	6.524	16.600	7.381	1.00	78.07	C
ATOM	171	CA	PRO	A	553	7.528	18.515	8.475	1.00	78.64	C
ATOM	172	CB	PRO	A	553	8.340	17.246	8.724	1.00	78.33	C
ATOM	173	CG	PRO	A	553	7.318	16.166	8.598	1.00	78.15	C
ATOM	174	C	PRO	A	553	8.389	19.673	7.963	1.00	78.40	C
ATOM	175	O	PRO	A	553	8.897	19.640	6.835	1.00	78.68	O
ATOM	176	N	ASP	A	554	8.545	20.700	8.795	1.00	77.55	N
ATOM	177	CA	ASP	A	554	9.352	21.854	8.415	1.00	76.93	C
ATOM	178	CB	ASP	A	554	9.151	23.023	9.393	1.00	76.00	C
ATOM	179	CG	ASP	A	554	7.820	23.721	9.196	1.00	76.42	C
ATOM	180	OD1	ASP	A	554	6.809	23.291	9.801	1.00	76.75	O
ATOM	181	OD2	ASP	A	554	7.785	24.693	8.414	1.00	74.81	O
ATOM	182	C	ASP	A	554	10.836	21.536	8.325	1.00	76.23	C
ATOM	183	O	ASP	A	554	11.451	21.123	9.301	1.00	76.48	O
ATOM	184	N	SER	A	555	11.400	21.731	7.138	1.00	76.12	N
ATOM	185	CA	SER	A	555	12.824	21.505	6.902	1.00	76.05	C
ATOM	186	CB	SER	A	555	13.019	20.492	5.767	1.00	76.21	C
ATOM	187	OG	SER	A	555	11.918	19.605	5.671	1.00	77.67	O
ATOM	188	C	SER	A	555	13.479	22.831	6.494	1.00	74.61	C
ATOM	189	O	SER	A	555	12.861	23.656	5.829	1.00	74.88	O
ATOM	190	N	THR	A	556	14.724	23.042	6.890	1.00	73.27	N
ATOM	191	CA	THR	A	556	15.414	24.264	6.505	1.00	72.06	C
ATOM	192	CB	THR	A	556	16.785	24.335	7.176	1.00	72.01	C
ATOM	193	OG1	THR	A	556	16.602	24.315	8.598	1.00	70.90	O
ATOM	194	CG2	THR	A	556	17.551	25.594	6.742	1.00	71.77	C
ATOM	195	C	THR	A	556	15.600	24.275	4.982	1.00	71.67	C
ATOM	196	O	THR	A	556	15.749	25.330	4.375	1.00	71.94	O
ATOM	197	N	TRP	A	557	15.595	23.096	4.369	1.00	70.39	N
ATOM	198	CA	TRP	A	557	15.762	22.993	2.924	1.00	69.47	C
ATOM	199	CB	TRP	A	557	16.278	21.603	2.558	1.00	69.26	C
ATOM	200	CG	TRP	A	557	15.879	21.140	1.192	1.00	68.51	C
ATOM	201	CD2	TRP	A	557	16.674	21.203	0.007	1.00	68.81	C
ATOM	202	CE2	TRP	A	557	15.899	20.666	-1.047	1.00	69.20	C
ATOM	203	CE3	TRP	A	557	17.969	21.662	-0.274	1.00	68.89	C
ATOM	204	CD1	TRP	A	557	14.683	20.583	0.825	1.00	68.76	C
ATOM	205	NE1	TRP	A	557	14.687	20.294	-0.519	1.00	69.36	N
ATOM	206	CZ2	TRP	A	557	16.377	20.573	-2.360	1.00	69.52	C
ATOM	207	CZ3	TRP	A	557	18.446	21.570	-1.580	1.00	69.22	C
ATOM	208	CH2	TRP	A	557	17.650	21.029	-2.606	1.00	69.23	C
ATOM	209	C	TRP	A	557	14.433	23.256	2.237	1.00	69.42	C
ATOM	210	O	TRP	A	557	14.377	23.845	1.156	1.00	69.20	O
ATOM	211	N	ARG	A	558	13.361	22.793	2.869	1.00	69.45	N
ATOM	212	CA	ARG	A	558	12.024	22.987	2.331	1.00	68.61	C
ATOM	213	CB	ARG	A	558	11.006	22.156	3.117	1.00	71.05	C
ATOM	214	CG	ARG	A	558	11.152	20.657	2.926	1.00	74.42	C
ATOM	215	CD	ARG	A	558	10.911	20.265	1.463	1.00	77.47	C
ATOM	216	NE	ARG	A	558	10.942	18.810	1.250	1.00	79.35	N
ATOM	217	CZ	ARG	A	558	10.789	18.200	0.071	1.00	79.72	C
ATOM	218	NH1	ARG	A	558	10.596	18.902	-1.042	1.00	79.73	N
ATOM	219	NH2	ARG	A	558	10.806	16.875	0.006	1.00	77.99	N
ATOM	220	C	ARG	A	558	11.656	24.468	2.406	1.00	66.30	C
ATOM	221	O	ARG	A	558	10.778	24.936	1.683	1.00	66.38	O
ATOM	222	N	ILE	A	559	12.332	25.205	3.284	1.00	62.72	N
ATOM	223	CA	ILE	A	559	12.067	26.633	3.431	1.00	60.06	C
ATOM	224	CB	ILE	A	559	12.234	27.084	4.904	1.00	58.16	C
ATOM	225	CG2	ILE	A	559	12.132	28.597	5.005	1.00	57.79	C
ATOM	226	CG1	ILE	A	559	11.153	26.442	5.771	1.00	55.84	C
ATOM	227	CD1	ILE	A	559	11.374	26.641	7.237	1.00	54.57	C
ATOM	228	C	ILE	A	559	12.989	27.466	2.528	1.00	58.90	C
ATOM	229	O	ILE	A	559	12.539	28.386	1.840	1.00	58.71	O
ATOM	230	N	MET	A	560	14.278	27.140	2.525	1.00	57.11	N
ATOM	231	CA	MET	A	560	15.215	27.879	1.687	1.00	55.49	C

ATOM	232	CB	MET	A	560	16.663	27.429	1.942	1.00	55.07	C
ATOM	233	CG	MET	A	560	17.279	27.911	3.261	1.00	55.01	C
ATOM	234	SD	MET	A	560	16.722	29.565	3.742	1.00	55.71	S
ATOM	235	CE	MET	A	560	17.693	30.607	2.615	1.00	56.88	C
ATOM	236	C	MET	A	560	14.866	27.671	0.215	1.00	53.30	C
ATOM	237	O	MET	A	560	15.039	28.562	-0.618	1.00	53.24	O
ATOM	238	N	THR	A	561	14.359	26.489	-0.101	1.00	51.46	N
ATOM	239	CA	THR	A	561	14.008	26.184	-1.472	1.00	49.42	C
ATOM	240	CB	THR	A	561	13.645	24.723	-1.614	1.00	47.12	C
ATOM	241	OG1	THR	A	561	14.833	23.955	-1.436	1.00	43.30	O
ATOM	242	CG2	THR	A	561	13.025	24.438	-2.992	1.00	47.09	C
ATOM	243	C	THR	A	561	12.847	27.035	-1.896	1.00	50.35	C
ATOM	244	O	THR	A	561	12.962	27.856	-2.813	1.00	49.29	O
ATOM	245	N	THR	A	562	11.729	26.829	-1.209	1.00	50.60	N
ATOM	246	CA	THR	A	562	10.513	27.566	-1.480	1.00	50.50	C
ATOM	247	CB	THR	A	562	9.410	27.243	-0.438	1.00	50.72	C
ATOM	248	OG1	THR	A	562	9.417	25.835	-0.181	1.00	49.04	O
ATOM	249	CG2	THR	A	562	8.015	27.654	-0.977	1.00	51.29	C
ATOM	250	C	THR	A	562	10.822	29.055	-1.441	1.00	50.76	C
ATOM	251	O	THR	A	562	10.295	29.810	-2.257	1.00	52.50	O
ATOM	252	N	LEU	A	563	11.679	29.466	-0.502	1.00	48.08	N
ATOM	253	CA	LEU	A	563	12.070	30.864	-0.377	1.00	48.07	C
ATOM	254	CB	LEU	A	563	12.976	31.093	0.842	1.00	48.05	C
ATOM	255	CG	LEU	A	563	12.321	31.685	2.096	1.00	47.81	C
ATOM	256	CD1	LEU	A	563	13.369	31.898	3.145	1.00	47.59	C
ATOM	257	CD2	LEU	A	563	11.680	33.009	1.794	1.00	48.28	C
ATOM	258	C	LEU	A	563	12.807	31.296	-1.628	1.00	49.19	C
ATOM	259	O	LEU	A	563	12.795	32.461	-2.010	1.00	49.29	O
ATOM	260	N	ASN	A	564	13.448	30.344	-2.280	1.00	50.80	N
ATOM	261	CA	ASN	A	564	14.172	30.660	-3.493	1.00	51.91	C
ATOM	262	CB	ASN	A	564	15.175	29.551	-3.759	1.00	54.20	C
ATOM	263	CG	ASN	A	564	16.105	29.865	-4.904	1.00	55.56	C
ATOM	264	OD1	ASN	A	564	15.709	29.854	-6.078	1.00	56.75	O
ATOM	265	ND2	ASN	A	564	17.358	30.142	-4.572	1.00	54.82	N
ATOM	266	C	ASN	A	564	13.228	30.842	-4.690	1.00	51.59	C
ATOM	267	O	ASN	A	564	13.363	31.786	-5.471	1.00	52.16	O
ATOM	268	N	MET	A	565	12.273	29.928	-4.831	1.00	49.72	N
ATOM	269	CA	MET	A	565	11.306	29.990	-5.922	1.00	48.12	C
ATOM	270	CB	MET	A	565	10.313	28.830	-5.803	1.00	50.29	C
ATOM	271	CG	MET	A	565	10.509	27.757	-6.866	1.00	54.07	C
ATOM	272	SD	MET	A	565	12.238	27.296	-7.119	1.00	59.68	S
ATOM	273	CE	MET	A	565	12.668	28.291	-8.568	1.00	56.89	C
ATOM	274	C	MET	A	565	10.575	31.332	-5.875	1.00	46.21	C
ATOM	275	O	MET	A	565	10.391	32.007	-6.896	1.00	44.66	O
ATOM	276	N	LEU	A	566	10.183	31.717	-4.665	1.00	42.77	N
ATOM	277	CA	LEU	A	566	9.476	32.967	-4.446	1.00	40.42	C
ATOM	278	CB	LEU	A	566	8.921	33.025	-3.012	1.00	39.77	C
ATOM	279	CG	LEU	A	566	8.272	34.368	-2.593	1.00	39.92	C
ATOM	280	CD1	LEU	A	566	7.049	34.700	-3.465	1.00	40.30	C
ATOM	281	CD2	LEU	A	566	7.871	34.309	-1.130	1.00	38.27	C
ATOM	282	C	LEU	A	566	10.398	34.166	-4.698	1.00	40.14	C
ATOM	283	O	LEU	A	566	10.027	35.113	-5.405	1.00	39.63	O
ATOM	284	N	GLY	A	567	11.597	34.100	-4.122	1.00	37.86	N
ATOM	285	CA	GLY	A	567	12.572	35.161	-4.248	1.00	35.66	C
ATOM	286	C	GLY	A	567	12.774	35.611	-5.678	1.00	37.12	C
ATOM	287	O	GLY	A	567	13.036	36.787	-5.952	1.00	35.69	O
ATOM	288	N	GLY	A	568	12.645	34.661	-6.597	1.00	37.04	N
ATOM	289	CA	GLY	A	568	12.800	34.960	-8.005	1.00	36.19	C
ATOM	290	C	GLY	A	568	11.627	35.756	-8.541	1.00	35.62	C
ATOM	291	O	GLY	A	568	11.782	36.847	-9.107	1.00	37.61	O
ATOM	292	N	ARG	A	569	10.433	35.213	-8.355	1.00	35.12	N
ATOM	293	CA	ARG	A	569	9.222	35.870	-8.819	1.00	34.25	C
ATOM	294	CB	ARG	A	569	8.006	35.053	-8.375	1.00	33.11	C
ATOM	295	CG	ARG	A	569	7.969	33.634	-8.925	1.00	31.46	C
ATOM	296	CD	ARG	A	569	7.066	32.772	-8.063	1.00	32.87	C
ATOM	297	NE	ARG	A	569	5.673	33.209	-8.075	1.00	34.06	N
ATOM	298	CZ	ARG	A	569	4.850	33.070	-7.040	1.00	33.79	C
ATOM	299	NH1	ARG	A	569	5.289	32.507	-5.923	1.00	35.27	N
ATOM	300	NH2	ARG	A	569	3.602	33.509	-7.106	1.00	31.40	N
ATOM	301	C	ARG	A	569	9.133	37.316	-8.297	1.00	33.11	C
ATOM	302	O	ARG	A	569	8.602	38.205	-8.971	1.00	32.54	O
ATOM	303	N	GLN	A	570	9.664	37.545	-7.098	1.00	30.74	N
ATOM	304	CA	GLN	A	570	9.669	38.883	-6.518	1.00	30.52	C
ATOM	305	CB	GLN	A	570	10.214	38.863	-5.104	1.00	29.10	C
ATOM	306	CG	GLN	A	570	9.645	37.808	-4.228	1.00	34.13	C
ATOM	307	CD	GLN	A	570	9.167	38.377	-2.927	1.00	36.47	C
ATOM	308	OE1	GLN	A	570	9.825	39.230	-2.318	1.00	36.20	O
ATOM	309	NE2	GLN	A	570	8.014	37.909	-2.483	1.00	38.29	N
ATOM	310	C	GLN	A	570	10.536	39.854	-7.322	1.00	31.59	C
ATOM	311	O	GLN	A	570	10.178	41.023	-7.479	1.00	30.59	O
ATOM	312	N	VAL	A	571	11.685	39.381	-7.801	1.00	32.05	N

ATOM	313	CA	VAL	A	571	12.581	40.241	-8.555	1.00	33.03	C
ATOM	314	CB	VAL	A	571	13.891	39.518	-8.979	1.00	33.17	C
ATOM	315	CG1	VAL	A	571	14.764	40.481	-9.786	1.00	28.63	C
ATOM	316	CG2	VAL	A	571	14.636	38.986	-7.748	1.00	32.83	C
ATOM	317	C	VAL	A	571	11.854	40.680	-9.811	1.00	35.62	C
ATOM	318	O	VAL	A	571	11.850	41.865	-10.155	1.00	36.48	O
ATOM	319	N	ILE	A	572	11.217	39.716	-10.476	1.00	34.39	N
ATOM	320	CA	ILE	A	572	10.472	39.975	-11.711	1.00	31.63	C
ATOM	321	CB	ILE	A	572	9.883	38.641	-12.289	1.00	30.51	C
ATOM	322	CG2	ILE	A	572	8.936	38.929	-13.450	1.00	26.00	C
ATOM	323	CG1	ILE	A	572	11.029	37.708	-12.727	1.00	27.62	C
ATOM	324	CD1	ILE	A	572	10.567	36.301	-13.094	1.00	25.32	C
ATOM	325	C	ILE	A	572	9.355	40.973	-11.398	1.00	30.52	C
ATOM	326	O	ILE	A	572	9.087	41.929	-12.145	1.00	30.96	O
ATOM	327	N	ALA	A	573	8.738	40.773	-10.246	1.00	29.17	N
ATOM	328	CA	ALA	A	573	7.662	41.648	-9.850	1.00	30.66	C
ATOM	329	CB	ALA	A	573	6.999	41.132	-8.584	1.00	23.83	C
ATOM	330	C	ALA	A	573	8.209	43.051	-9.652	1.00	32.75	C
ATOM	331	O	ALA	A	573	7.697	44.009	-10.245	1.00	34.65	O
ATOM	332	N	ALA	A	574	9.246	43.171	-8.824	1.00	34.21	N
ATOM	333	CA	ALA	A	574	9.893	44.457	-8.547	1.00	35.99	C
ATOM	334	CB	ALA	A	574	11.082	44.242	-7.576	1.00	37.77	C
ATOM	335	C	ALA	A	574	10.380	45.104	-9.863	1.00	35.89	C
ATOM	336	O	ALA	A	574	10.450	46.334	-9.985	1.00	34.82	O
ATOM	337	N	VAL	A	575	10.695	44.270	-10.849	1.00	34.71	N
ATOM	338	CA	VAL	A	575	11.137	44.773	-12.140	1.00	36.38	C
ATOM	339	CB	VAL	A	575	11.758	43.632	-13.016	1.00	37.23	C
ATOM	340	CG1	VAL	A	575	11.901	44.076	-14.479	1.00	36.32	C
ATOM	341	CG2	VAL	A	575	13.136	43.279	-12.490	1.00	38.27	C
ATOM	342	C	VAL	A	575	9.966	45.403	-12.885	1.00	37.14	C
ATOM	343	O	VAL	A	575	10.113	46.448	-13.518	1.00	37.37	O
ATOM	344	N	LYS	A	576	8.805	44.764	-12.815	1.00	37.85	N
ATOM	345	CA	LYS	A	576	7.617	45.280	-13.485	1.00	38.77	C
ATOM	346	CB	LYS	A	576	6.506	44.236	-13.429	1.00	39.36	C
ATOM	347	CG	LYS	A	576	5.360	44.562	-14.334	1.00	43.51	C
ATOM	348	CD	LYS	A	576	4.079	43.877	-13.916	1.00	46.79	C
ATOM	349	CE	LYS	A	576	2.877	44.781	-14.236	1.00	48.91	C
ATOM	350	NZ	LYS	A	576	3.034	46.142	-13.588	1.00	48.36	N
ATOM	351	C	LYS	A	576	7.158	46.544	-12.760	1.00	39.15	C
ATOM	352	O	LYS	A	576	6.753	47.537	-13.364	1.00	39.95	O
ATOM	353	N	TRP	A	577	7.232	46.502	-11.445	1.00	36.56	N
ATOM	354	CA	TRP	A	577	6.819	47.638	-10.678	1.00	36.07	C
ATOM	355	CB	TRP	A	577	6.961	47.318	-9.202	1.00	33.65	C
ATOM	356	CG	TRP	A	577	6.970	48.528	-8.339	1.00	31.88	C
ATOM	357	CD2	TRP	A	577	8.127	49.185	-7.764	1.00	31.22	C
ATOM	358	CE2	TRP	A	577	7.641	50.253	-6.973	1.00	29.27	C
ATOM	359	CE3	TRP	A	577	9.517	48.973	-7.840	1.00	28.86	C
ATOM	360	CD1	TRP	A	577	5.880	49.212	-7.894	1.00	30.51	C
ATOM	361	NE1	TRP	A	577	6.277	50.243	-7.072	1.00	31.72	N
ATOM	362	CZ2	TRP	A	577	8.495	51.111	-6.250	1.00	28.61	C
ATOM	363	CZ3	TRP	A	577	10.377	49.845	-7.108	1.00	27.76	C
ATOM	364	CH2	TRP	A	577	9.852	50.891	-6.329	1.00	27.24	C
ATOM	365	C	TRP	A	577	7.653	48.865	-11.032	1.00	37.91	C
ATOM	366	O	TRP	A	577	7.131	49.972	-11.208	1.00	36.99	O
ATOM	367	N	ALA	A	578	8.961	48.664	-11.156	1.00	40.51	N
ATOM	368	CA	ALA	A	578	9.860	49.774	-11.478	1.00	41.65	C
ATOM	369	CB	ALA	A	578	11.304	49.287	-11.532	1.00	40.34	C
ATOM	370	C	ALA	A	578	9.465	50.438	-12.796	1.00	41.28	C
ATOM	371	O	ALA	A	578	9.384	51.661	-12.885	1.00	39.86	O
ATOM	372	N	LYS	A	579	9.216	49.624	-13.814	1.00	43.04	N
ATOM	373	CA	LYS	A	579	8.847	50.146	-15.120	1.00	46.65	C
ATOM	374	CB	LYS	A	579	8.614	48.996	-16.107	1.00	46.24	C
ATOM	375	CG	LYS	A	579	9.851	48.195	-16.466	1.00	46.67	C
ATOM	376	CD	LYS	A	579	9.897	47.962	-17.957	1.00	48.01	C
ATOM	377	CE	LYS	A	579	11.324	48.069	-18.494	1.00	50.77	C
ATOM	378	NZ	LYS	A	579	11.402	48.236	-19.987	1.00	47.84	N
ATOM	379	C	LYS	A	579	7.593	51.024	-15.046	1.00	49.17	C
ATOM	380	O	LYS	A	579	7.457	51.994	-15.801	1.00	50.93	O
ATOM	381	N	ALA	A	580	6.695	50.696	-14.120	1.00	49.47	N
ATOM	382	CA	ALA	A	580	5.446	51.421	-13.948	1.00	48.74	C
ATOM	383	CB	ALA	A	580	4.459	50.570	-13.138	1.00	47.63	C
ATOM	384	C	ALA	A	580	5.675	52.764	-13.274	1.00	50.11	C
ATOM	385	O	ALA	A	580	4.873	53.686	-13.436	1.00	51.36	O
ATOM	386	N	ILE	A	581	6.772	52.885	-12.531	1.00	51.42	N
ATOM	387	CA	ILE	A	581	7.107	54.142	-11.848	1.00	51.19	C
ATOM	388	CB	ILE	A	581	8.472	54.049	-11.087	1.00	51.78	C
ATOM	389	CG2	ILE	A	581	8.701	55.323	-10.292	1.00	51.98	C
ATOM	390	CG1	ILE	A	581	8.499	52.836	-10.146	1.00	50.73	C
ATOM	391	CD1	ILE	A	581	7.537	52.921	-8.983	1.00	49.50	C
ATOM	392	C	ILE	A	581	7.204	55.278	-12.873	1.00	51.72	C
ATOM	393	O	ILE	A	581	7.993	55.224	-13.813	1.00	51.09	O

ATOM	394	N	PRO A 582	6.385	56.323	-12.704	1.00	54.02	N
ATOM	395	CD	PRO A 582	5.345	56.458	-11.670	1.00	52.87	C
ATOM	396	CA	PRO A 582	6.370	57.479	-13.608	1.00	54.01	C
ATOM	397	CB	PRO A 582	5.405	58.437	-12.917	1.00	54.01	C
ATOM	398	CG	PRO A 582	4.442	57.501	-12.261	1.00	53.51	C
ATOM	399	C	PRO A 582	7.747	58.115	-13.824	1.00	54.80	O
ATOM	400	O	PRO A 582	8.366	58.607	-12.881	1.00	53.81	N
ATOM	401	N	GLY A 583	8.215	58.087	-15.070	1.00	55.74	C
ATOM	402	CA	GLY A 583	9.491	58.688	-15.403	1.00	56.81	C
ATOM	403	C	GLY A 583	10.634	57.704	-15.430	1.00	57.67	O
ATOM	404	O	GLY A 583	11.714	58.003	-15.947	1.00	58.72	N
ATOM	405	N	PHE A 584	10.404	56.525	-14.866	1.00	56.97	C
ATOM	406	CA	PHE A 584	11.432	55.496	-14.833	1.00	56.64	C
ATOM	407	CB	PHE A 584	10.960	54.282	-14.010	1.00	52.95	C
ATOM	408	CG	PHE A 584	12.009	53.206	-13.854	1.00	49.47	C
ATOM	409	CD1	PHE A 584	13.078	53.371	-12.978	1.00	47.44	C
ATOM	410	CD2	PHE A 584	11.957	52.052	-14.611	1.00	47.12	C
ATOM	411	CE1	PHE A 584	14.067	52.409	-12.867	1.00	44.97	C
ATOM	412	CE2	PHE A 584	12.947	51.094	-14.494	1.00	46.11	C
ATOM	413	CZ	PHE A 584	14.002	51.279	-13.622	1.00	44.16	C
ATOM	414	C	PHE A 584	11.803	55.038	-16.247	1.00	58.50	O
ATOM	415	O	PHE A 584	12.984	54.860	-16.563	1.00	58.64	N
ATOM	416	N	ARG A 585	10.790	54.849	-17.091	1.00	60.26	C
ATOM	417	CA	ARG A 585	11.007	54.393	-18.463	1.00	61.00	C
ATOM	418	CB	ARG A 585	9.703	53.875	-19.073	1.00	60.88	C
ATOM	419	CG	ARG A 585	9.687	52.380	-19.352	1.00	62.71	C
ATOM	420	CD	ARG A 585	8.268	51.908	-19.644	1.00	64.91	N
ATOM	421	NE	ARG A 585	8.171	50.458	-19.777	1.00	67.64	C
ATOM	422	CZ	ARG A 585	8.412	49.782	-20.899	1.00	70.40	N
ATOM	423	NH1	ARG A 585	8.761	50.425	-22.005	1.00	70.62	N
ATOM	424	NH2	ARG A 585	8.316	48.454	-20.916	1.00	70.06	C
ATOM	425	C	ARG A 585	11.585	55.494	-19.330	1.00	61.90	O
ATOM	426	O	ARG A 585	11.965	55.250	-20.469	1.00	61.35	N
ATOM	427	N	ASN A 586	11.646	56.705	-18.780	1.00	63.51	C
ATOM	428	CA	ASN A 586	12.207	57.860	-19.488	1.00	64.69	C
ATOM	429	CB	ASN A 586	11.563	59.152	-18.980	1.00	65.67	C
ATOM	430	CG	ASN A 586	10.107	59.266	-19.376	1.00	67.09	O
ATOM	431	OD1	ASN A 586	9.381	60.157	-18.917	1.00	66.96	N
ATOM	432	ND2	ASN A 586	9.669	58.362	-20.243	1.00	66.08	C
ATOM	433	C	ASN A 586	13.728	57.937	-19.305	1.00	64.75	O
ATOM	434	O	ASN A 586	14.407	58.745	-19.954	1.00	65.61	N
ATOM	435	N	LEU A 587	14.246	57.108	-18.398	1.00	63.05	C
ATOM	436	CA	LEU A 587	15.677	57.034	-18.114	1.00	61.56	C
ATOM	437	CB	LEU A 587	15.916	56.338	-16.766	1.00	59.73	C
ATOM	438	CG	LEU A 587	15.159	56.892	-15.557	1.00	58.39	C
ATOM	439	CD1	LEU A 587	15.295	55.945	-14.379	1.00	54.35	C
ATOM	440	CD2	LEU A 587	15.690	58.276	-15.212	1.00	59.13	C
ATOM	441	C	LEU A 587	16.346	56.229	-19.227	1.00	62.41	O
ATOM	442	O	LEU A 587	15.688	55.460	-19.940	1.00	61.86	N
ATOM	443	N	HIS A 588	17.652	56.413	-19.385	1.00	63.82	C
ATOM	444	CA	HIS A 588	18.395	55.691	-20.407	1.00	64.92	C
ATOM	445	CB	HIS A 588	19.878	56.080	-20.363	1.00	66.72	C
ATOM	446	CG	HIS A 588	20.631	55.740	-21.614	1.00	69.11	C
ATOM	447	CD2	HIS A 588	20.414	54.802	-22.567	1.00	69.77	N
ATOM	448	ND1	HIS A 588	21.767	56.422	-22.004	1.00	69.86	C
ATOM	449	CE1	HIS A 588	22.212	55.915	-23.144	1.00	70.16	N
ATOM	450	NE2	HIS A 588	21.407	54.931	-23.504	1.00	69.84	C
ATOM	451	C	HIS A 588	18.211	54.200	-20.140	1.00	65.56	O
ATOM	452	O	HIS A 588	18.124	53.758	-18.993	1.00	64.81	N
ATOM	453	N	LEU A 589	18.153	53.426	-21.209	1.00	66.84	C
ATOM	454	CA	LEU A 589	17.932	52.002	-21.088	1.00	68.00	C
ATOM	455	CB	LEU A 589	17.742	51.403	-22.478	1.00	67.58	C
ATOM	456	CG	LEU A 589	16.982	50.088	-22.566	1.00	67.32	C
ATOM	457	CD1	LEU A 589	15.608	50.271	-21.917	1.00	65.32	C
ATOM	458	CD2	LEU A 589	16.874	49.660	-24.039	1.00	67.70	C
ATOM	459	C	LEU A 589	19.037	51.258	-20.361	1.00	69.34	O
ATOM	460	O	LEU A 589	18.844	50.113	-19.962	1.00	70.96	N
ATOM	461	N	ASP A 590	20.189	51.897	-20.179	1.00	70.21	C
ATOM	462	CA	ASP A 590	21.314	51.235	-19.521	1.00	69.58	C
ATOM	463	CB	ASP A 590	22.660	51.769	-20.067	1.00	70.15	C
ATOM	464	CG	ASP A 590	22.537	52.430	-21.456	1.00	71.99	O
ATOM	465	OD1	ASP A 590	21.855	51.877	-22.336	1.00	72.17	O
ATOM	466	OD2	ASP A 590	23.140	53.507	-21.683	1.00	73.93	C
ATOM	467	C	ASP A 590	21.253	51.428	-18.009	1.00	68.21	O
ATOM	468	O	ASP A 590	21.090	50.473	-17.247	1.00	67.71	N
ATOM	469	N	ASP A 591	21.370	52.677	-17.582	1.00	68.04	C
ATOM	470	CA	ASP A 591	21.358	52.997	-16.164	1.00	67.55	C
ATOM	471	CB	ASP A 591	21.624	54.502	-15.980	1.00	68.82	C
ATOM	472	CG	ASP A 591	20.562	55.355	-16.617	1.00	68.52	O
ATOM	473	OD1	ASP A 591	20.665	56.606	-16.558	1.00	68.25	O
ATOM	474	OD2	ASP A 591	19.621	54.749	-17.173	1.00	68.72	O



ATOM	556	C	TRP	A	600	16.149	44.045	-4.655	1.00	40.84	C
ATOM	557	O	TRP	A	600	15.100	43.639	-4.144	1.00	42.57	O
ATOM	558	N	MET	A	601	17.318	43.964	-4.030	1.00	40.62	N
ATOM	559	CA	MET	A	601	17.370	43.383	-2.700	1.00	37.96	C
ATOM	560	CB	MET	A	601	18.789	42.874	-2.367	1.00	39.10	C
ATOM	561	CG	MET	A	601	18.951	42.285	-0.929	1.00	36.78	C
ATOM	562	SD	MET	A	601	17.661	41.045	-0.407	1.00	38.16	S
ATOM	563	CE	MET	A	601	18.412	39.458	-0.893	1.00	28.58	C
ATOM	564	C	MET	A	601	16.897	44.410	-1.673	1.00	35.33	C
ATOM	565	O	MET	A	601	16.415	44.031	-0.618	1.00	33.40	O
ATOM	566	N	PHE	A	602	17.026	45.700	-1.985	1.00	33.32	N
ATOM	567	CA	PHE	A	602	16.558	46.767	-1.087	1.00	33.61	C
ATOM	568	CB	PHE	A	602	16.990	48.133	-1.615	1.00	32.68	C
ATOM	569	CG	PHE	A	602	18.413	48.488	-1.304	1.00	35.07	C
ATOM	570	CD1	PHE	A	602	19.471	48.026	-2.099	1.00	34.67	C
ATOM	571	CD2	PHE	A	602	18.699	49.286	-0.203	1.00	35.29	C
ATOM	572	CE1	PHE	A	602	20.803	48.368	-1.796	1.00	35.82	C
ATOM	573	CE2	PHE	A	602	20.020	49.637	0.120	1.00	36.29	C
ATOM	574	CZ	PHE	A	602	21.079	49.177	-0.677	1.00	36.30	C
ATOM	575	C	PHE	A	602	15.018	46.743	-1.013	1.00	34.19	C
ATOM	576	O	PHE	A	602	14.411	46.843	0.053	1.00	32.90	O
ATOM	577	N	LEU	A	603	14.412	46.622	-2.186	1.00	34.93	N
ATOM	578	CA	LEU	A	603	12.970	46.578	-2.351	1.00	33.13	C
ATOM	579	CB	LEU	A	603	12.657	46.535	-3.853	1.00	30.04	C
ATOM	580	CG	LEU	A	603	13.307	47.603	-4.746	1.00	26.04	C
ATOM	581	CD1	LEU	A	603	13.088	47.232	-6.235	1.00	18.93	C
ATOM	582	CD2	LEU	A	603	12.749	49.002	-4.344	1.00	21.25	C
ATOM	583	C	LEU	A	603	12.368	45.347	-1.657	1.00	34.15	C
ATOM	584	O	LEU	A	603	11.654	45.452	-0.648	1.00	34.86	O
ATOM	585	N	MET	A	604	12.672	44.173	-2.207	1.00	34.03	N
ATOM	586	CA	MET	A	604	12.161	42.908	-1.667	1.00	33.17	C
ATOM	587	CB	MET	A	604	12.904	41.733	-2.292	1.00	31.37	C
ATOM	588	CG	MET	A	604	12.639	41.605	-3.770	1.00	31.35	C
ATOM	589	SD	MET	A	604	13.532	40.260	-4.533	1.00	34.84	S
ATOM	590	CE	MET	A	604	13.049	38.828	-3.435	1.00	32.50	C
ATOM	591	C	MET	A	604	12.274	42.848	-0.151	1.00	34.90	C
ATOM	592	O	MET	A	604	11.353	42.395	0.549	1.00	34.42	O
ATOM	593	N	ALA	A	605	13.411	43.314	0.356	1.00	35.16	N
ATOM	594	CA	ALA	A	605	13.645	43.314	1.797	1.00	35.75	C
ATOM	595	CB	ALA	A	605	15.167	43.549	2.115	1.00	34.01	C
ATOM	596	C	ALA	A	605	12.790	44.357	2.522	1.00	35.26	C
ATOM	597	O	ALA	A	605	12.267	44.088	3.603	1.00	35.64	O
ATOM	598	N	PHE	A	606	12.657	45.543	1.936	1.00	34.31	N
ATOM	599	CA	PHE	A	606	11.880	46.608	2.554	1.00	33.65	C
ATOM	600	CB	PHE	A	606	12.104	47.924	1.790	1.00	32.95	C
ATOM	601	CG	PHE	A	606	11.632	49.141	2.526	1.00	31.43	C
ATOM	602	CD1	PHE	A	606	12.130	49.443	3.782	1.00	28.25	C
ATOM	603	CD2	PHE	A	606	10.652	49.971	1.974	1.00	32.65	C
ATOM	604	CE1	PHE	A	606	11.658	50.546	4.485	1.00	26.61	C
ATOM	605	CE2	PHE	A	606	10.168	51.084	2.671	1.00	30.07	C
ATOM	606	CZ	PHE	A	606	10.669	51.370	3.923	1.00	29.38	C
ATOM	607	C	PHE	A	606	10.411	46.196	2.525	1.00	34.29	C
ATOM	608	O	PHE	A	606	9.642	46.502	3.438	1.00	33.41	O
ATOM	609	N	ALA	A	607	10.037	45.468	1.480	1.00	35.25	N
ATOM	610	CA	ALA	A	607	8.665	45.009	1.366	1.00	36.22	C
ATOM	611	CB	ALA	A	607	8.403	44.452	-0.017	1.00	36.17	C
ATOM	612	C	ALA	A	607	8.402	43.946	2.425	1.00	36.85	C
ATOM	613	O	ALA	A	607	7.380	43.999	3.095	1.00	37.58	O
ATOM	614	N	LEU	A	608	9.321	42.989	2.562	1.00	36.93	N
ATOM	615	CA	LEU	A	608	9.211	41.926	3.557	1.00	38.22	C
ATOM	616	CB	LEU	A	608	10.444	41.008	3.513	1.00	40.70	C
ATOM	617	CG	LEU	A	608	10.649	40.006	4.669	1.00	40.62	C
ATOM	618	CD1	LEU	A	608	9.509	39.016	4.612	1.00	40.77	C
ATOM	619	CD2	LEU	A	608	12.002	39.258	4.572	1.00	39.90	C
ATOM	620	C	LEU	A	608	9.135	42.541	4.942	1.00	38.61	C
ATOM	621	O	LEU	A	608	8.477	42.018	5.840	1.00	38.85	O
ATOM	622	N	GLY	A	609	9.819	43.653	5.137	1.00	39.17	N
ATOM	623	CA	GLY	A	609	9.766	44.237	6.451	1.00	40.69	C
ATOM	624	C	GLY	A	609	8.406	44.845	6.689	1.00	42.50	C
ATOM	625	O	GLY	A	609	7.921	44.876	7.817	1.00	44.18	O
ATOM	626	N	TRP	A	610	7.773	45.324	5.626	1.00	42.62	N
ATOM	627	CA	TRP	A	610	6.474	45.967	5.775	1.00	42.74	C
ATOM	628	CB	TRP	A	610	6.133	46.756	4.516	1.00	42.60	C
ATOM	629	CG	TRP	A	610	4.733	47.255	4.492	1.00	44.55	C
ATOM	630	CD2	TRP	A	610	4.205	48.403	5.179	1.00	45.24	C
ATOM	631	CE2	TRP	A	610	2.834	48.482	4.861	1.00	43.72	C
ATOM	632	CE3	TRP	A	610	4.763	49.371	6.033	1.00	47.28	C
ATOM	633	CD1	TRP	A	610	3.686	46.705	3.811	1.00	42.47	C
ATOM	634	NE1	TRP	A	610	2.548	47.434	4.027	1.00	43.12	N
ATOM	635	CZ2	TRP	A	610	1.999	49.488	5.361	1.00	44.90	C
ATOM	636	CZ3	TRP	A	610	3.922	50.382	6.536	1.00	48.40	C

ATOM	637	CH2	TRP	A	610	2.559	50.426	6.194	1.00	46.55	C
ATOM	638	C	TRP	A	610	5.399	44.944	6.076	1.00	41.95	C
ATOM	639	O	TRP	A	610	4.608	45.091	7.009	1.00	41.38	O
ATOM	640	N	ARG	A	611	5.378	43.891	5.282	1.00	40.58	N
ATOM	641	CA	ARG	A	611	4.404	42.846	5.491	1.00	41.03	C
ATOM	642	CB	ARG	A	611	4.605	41.755	4.451	1.00	35.31	C
ATOM	643	CG	ARG	A	611	4.206	42.164	3.053	1.00	31.56	C
ATOM	644	CD	ARG	A	611	4.033	40.923	2.181	1.00	31.17	C
ATOM	645	NE	ARG	A	611	5.255	40.145	2.164	1.00	32.10	N
ATOM	646	CZ	ARG	A	611	6.310	40.400	1.398	1.00	32.07	C
ATOM	647	NH1	ARG	A	611	6.305	41.413	0.531	1.00	32.40	N
ATOM	648	NH2	ARG	A	611	7.418	39.687	1.581	1.00	31.27	N
ATOM	649	C	ARG	A	611	4.498	42.242	6.903	1.00	43.13	C
ATOM	650	O	ARG	A	611	3.482	41.856	7.505	1.00	43.41	O
ATOM	651	N	SER	A	612	5.720	42.166	7.426	1.00	44.51	N
ATOM	652	CA	SER	A	612	5.950	41.595	8.750	1.00	46.13	C
ATOM	653	CB	SER	A	612	7.454	41.393	9.001	1.00	44.76	C
ATOM	654	OG	SER	A	612	7.949	40.301	8.249	1.00	44.54	O
ATOM	655	C	SER	A	612	5.365	42.494	9.822	1.00	46.95	C
ATOM	656	O	SER	A	612	4.573	42.054	10.651	1.00	47.60	O
ATOM	657	N	TYR	A	613	4.498	43.759	9.787	1.00	47.45	N
ATOM	658	CA	TYR	A	613	5.754	43.759	10.752	1.00	49.45	C
ATOM	659	CB	TYR	A	613	5.290	44.738	10.752	1.00	46.02	C
ATOM	660	CG	TYR	A	613	6.026	46.058	10.491	1.00	46.02	C
ATOM	661	CD1	TYR	A	613	5.230	47.308	10.749	1.00	39.72	C
ATOM	662	CE1	TYR	A	613	4.879	47.688	12.040	1.00	39.52	C
ATOM	663	CD2	TYR	A	613	4.159	48.855	12.267	1.00	38.96	C
ATOM	664	CE2	TYR	A	613	4.827	48.110	9.697	1.00	37.42	C
ATOM	665	CZ	TYR	A	613	4.115	49.266	9.913	1.00	36.61	C
ATOM	666	OH	TYR	A	613	3.779	49.635	11.193	1.00	37.44	O
ATOM	667	C	TYR	A	613	3.130	50.824	11.393	1.00	34.70	C
ATOM	668	O	TYR	A	613	3.784	44.948	10.656	1.00	52.41	O
ATOM	669	N	ARG	A	614	3.082	45.141	11.656	1.00	52.98	N
ATOM	670	CA	ARG	A	614	3.295	44.886	9.429	1.00	56.04	C
ATOM	671	CB	ARG	A	614	1.895	45.111	9.169	1.00	59.35	C
ATOM	672	CG	ARG	A	614	1.717	45.463	7.691	1.00	61.72	C
ATOM	673	CD	ARG	A	614	0.299	45.367	7.188	1.00	66.15	C
ATOM	674	NE	ARG	A	614	-0.201	46.679	6.575	1.00	69.45	N
ATOM	675	CZ	ARG	A	614	-0.274	47.765	7.553	1.00	69.96	C
ATOM	676	NH1	ARG	A	614	-1.038	48.846	7.421	1.00	69.24	N
ATOM	677	NH2	ARG	A	614	-1.806	49.014	6.345	1.00	66.17	N
ATOM	678	C	ARG	A	614	-1.062	49.741	8.399	1.00	69.78	C
ATOM	679	O	ARG	A	614	1.038	43.921	9.566	1.00	60.21	O
ATOM	680	N	GLN	A	615	-0.128	44.090	9.901	1.00	61.10	N
ATOM	681	CA	GLN	A	615	1.621	42.726	9.571	1.00	61.96	C
ATOM	682	CB	GLN	A	615	0.876	41.513	9.913	1.00	63.75	C
ATOM	683	CG	GLN	A	615	1.414	40.354	9.069	1.00	63.82	C
ATOM	684	CD	GLN	A	615	0.365	39.341	8.617	1.00	65.38	C
ATOM	685	OE1	GLN	A	615	0.181	38.212	9.612	1.00	67.72	O
ATOM	686	NE2	GLN	A	615	1.138	37.514	9.950	1.00	68.86	N
ATOM	687	C	GLN	A	615	-1.050	38.022	10.087	1.00	68.30	C
ATOM	688	O	GLN	A	615	0.937	41.185	11.414	1.00	64.87	O
ATOM	689	N	SER	A	616	0.104	40.432	11.927	1.00	64.17	N
ATOM	690	CA	SER	A	616	1.907	41.780	12.111	1.00	67.26	C
ATOM	691	CB	SER	A	616	2.096	41.547	13.545	1.00	68.99	C
ATOM	692	OG	SER	A	616	2.662	40.132	13.758	1.00	69.83	O
ATOM	693	C	SER	A	616	3.046	39.899	15.104	1.00	69.86	C
ATOM	694	O	SER	A	616	3.003	42.581	14.236	1.00	70.29	O
ATOM	695	N	SER	A	617	3.962	43.096	13.644	1.00	70.23	N
ATOM	696	CA	SER	A	617	2.681	42.872	15.495	1.00	71.63	C
ATOM	697	CB	SER	A	617	3.437	43.822	16.307	1.00	72.46	C
ATOM	698	OG	SER	A	617	2.488	44.879	16.914	1.00	73.51	O
ATOM	699	C	SER	A	617	1.875	45.694	15.908	1.00	74.66	C
ATOM	700	O	SER	A	617	4.176	43.043	17.404	1.00	72.58	O
ATOM	701	N	ALA	A	618	4.090	43.363	18.585	1.00	73.15	N
ATOM	702	CA	ALA	A	618	4.919	42.026	16.980	1.00	71.68	C
ATOM	703	CB	ALA	A	618	5.690	41.174	17.874	1.00	71.19	C
ATOM	704	C	ALA	A	618	4.798	40.687	19.050	1.00	71.51	C
ATOM	705	O	ALA	A	618	6.182	39.993	17.044	1.00	71.07	O
ATOM	706	N	ASN	A	619	5.415	39.458	16.251	1.00	71.64	N
ATOM	707	CA	ASN	A	619	7.464	39.635	17.200	1.00	70.12	C
ATOM	708	CB	ASN	A	619	8.100	38.512	16.486	1.00	68.44	C
ATOM	709	CG	ASN	A	619	7.525	37.149	16.939	1.00	70.83	O
ATOM	710	OD1	ASN	A	619	7.550	36.937	18.452	1.00	72.69	O
ATOM	711	ND2	ASN	A	619	8.504	37.315	19.136	1.00	73.24	N
ATOM	712	C	ASN	A	619	6.503	36.288	18.973	1.00	72.29	C
ATOM	713	O	ASN	A	619	7.820	38.610	15.001	1.00	66.42	O
ATOM	714	N	LEU	A	620	7.457	39.668	14.497	1.00	67.27	N
ATOM	715	CA	LEU	A	620	7.987	37.474	14.328	1.00	63.53	C
ATOM	716	CB	LEU	A	620	7.675	37.283	12.909	1.00	61.17	C
ATOM	717	CG	LEU	A	620	6.176	37.519	12.694	1.00	61.45	C
ATOM	717	CG	LEU	A	620	5.291	36.520	13.431	1.00	61.73	C

ATOM	718	CD1	LEU	A	620	3.846	36.973	13.422	1.00	61.94	C
ATOM	719	CD2	LEU	A	620	5.463	35.155	12.798	1.00	62.76	C
ATOM	720	C	LEU	A	620	8.386	37.899	11.722	1.00	59.14	C
ATOM	721	O	LEU	A	620	9.041	38.943	11.785	1.00	59.57	O
ATOM	722	N	LEU	A	621	8.195	37.194	10.615	1.00	56.65	N
ATOM	723	CA	LEU	A	621	8.708	37.540	9.307	1.00	55.25	C
ATOM	724	CB	LEU	A	621	10.045	36.859	9.023	1.00	56.50	C
ATOM	725	CG	LEU	A	621	11.339	37.679	9.165	1.00	58.03	C
ATOM	726	CD1	LEU	A	621	12.507	36.909	8.514	1.00	58.11	C
ATOM	727	CD2	LEU	A	621	11.169	39.058	8.510	1.00	55.91	C
ATOM	728	C	LEU	A	621	7.656	36.988	8.367	1.00	53.52	C
ATOM	729	O	LEU	A	621	7.488	35.775	8.267	1.00	50.87	O
ATOM	730	N	CYS	A	622	6.952	37.879	7.682	1.00	52.96	N
ATOM	731	CA	CYS	A	622	5.900	37.461	6.780	1.00	54.54	C
ATOM	732	CB	CYS	A	622	4.686	38.369	6.983	1.00	55.42	C
ATOM	733	SG	CYS	A	622	3.205	37.752	6.180	1.00	60.90	S
ATOM	734	C	CYS	A	622	6.314	37.425	5.302	1.00	54.09	C
ATOM	735	O	CYS	A	622	5.954	38.301	4.513	1.00	53.78	O
ATOM	736	N	PHE	A	623	7.062	36.392	4.924	1.00	55.17	N
ATOM	737	CA	PHE	A	623	7.519	36.257	3.542	1.00	56.37	C
ATOM	738	CB	PHE	A	623	8.329	34.979	3.371	1.00	55.59	C
ATOM	739	CG	PHE	A	623	9.616	34.982	4.118	1.00	57.62	C
ATOM	740	CD1	PHE	A	623	10.677	35.787	3.712	1.00	59.06	C
ATOM	741	CD2	PHE	A	623	9.772	34.178	5.240	1.00	57.97	C
ATOM	742	CE1	PHE	A	623	11.885	35.788	4.417	1.00	59.87	C
ATOM	743	CE2	PHE	A	623	10.965	34.168	5.956	1.00	57.83	C
ATOM	744	CZ	PHE	A	623	12.027	34.973	5.547	1.00	58.68	C
ATOM	745	C	PHE	A	623	6.335	36.241	2.595	1.00	56.58	C
ATOM	746	O	PHE	A	623	6.317	36.936	1.576	1.00	56.24	O
ATOM	747	N	ALA	A	624	5.348	35.433	2.958	1.00	58.43	N
ATOM	748	CA	ALA	A	624	4.128	35.291	2.191	1.00	58.80	C
ATOM	749	CB	ALA	A	624	4.317	34.258	1.117	1.00	59.29	C
ATOM	750	C	ALA	A	624	3.004	34.880	3.128	1.00	59.45	C
ATOM	751	O	ALA	A	624	3.240	34.339	4.218	1.00	60.17	O
ATOM	752	N	PRO	A	625	1.758	35.134	2.720	1.00	58.79	N
ATOM	753	CD	PRO	A	625	1.316	35.831	1.504	1.00	58.23	C
ATOM	754	CA	PRO	A	625	0.610	34.777	3.552	1.00	58.30	C
ATOM	755	CB	PRO	A	625	-0.574	35.130	2.655	1.00	58.44	C
ATOM	756	CG	PRO	A	625	-0.067	36.300	1.902	1.00	58.45	C
ATOM	757	C	PRO	A	625	0.602	33.312	3.990	1.00	57.40	C
ATOM	758	O	PRO	A	625	-0.045	32.962	4.973	1.00	56.41	O
ATOM	759	N	ASP	A	626	1.342	32.471	3.267	1.00	57.37	N
ATOM	760	CA	ASP	A	626	1.404	31.036	3.563	1.00	57.73	C
ATOM	761	CB	ASP	A	626	0.836	30.235	2.379	1.00	58.49	C
ATOM	762	CG	ASP	A	626	1.750	30.260	1.147	1.00	59.16	C
ATOM	763	OD1	ASP	A	626	2.320	31.328	0.839	1.00	59.10	O
ATOM	764	OD2	ASP	A	626	1.888	29.209	0.477	1.00	59.56	O
ATOM	765	C	ASP	A	626	2.820	30.554	3.873	1.00	57.51	C
ATOM	766	O	ASP	A	626	3.178	29.408	3.586	1.00	56.84	O
ATOM	767	N	LEU	A	627	3.622	31.436	4.455	1.00	57.58	N
ATOM	768	CA	LEU	A	627	4.994	31.094	4.793	1.00	58.80	C
ATOM	769	CB	LEU	A	627	5.868	31.002	3.537	1.00	57.66	C
ATOM	770	CG	LEU	A	627	7.313	30.521	3.726	1.00	55.56	C
ATOM	771	CD1	LEU	A	627	7.293	29.144	4.404	1.00	53.88	C
ATOM	772	CD2	LEU	A	627	8.040	30.466	2.365	1.00	55.45	C
ATOM	773	C	LEU	A	627	5.598	32.120	5.723	1.00	59.11	C
ATOM	774	O	LEU	A	627	6.565	32.792	5.366	1.00	59.97	O
ATOM	775	N	ILE	A	628	5.021	32.228	6.913	1.00	59.55	N
ATOM	776	CA	ILE	A	628	5.493	33.150	7.933	1.00	60.24	C
ATOM	777	CB	ILE	A	628	4.299	33.706	8.749	1.00	59.38	C
ATOM	778	CG2	ILE	A	628	4.716	34.959	9.522	1.00	59.44	C
ATOM	779	CG1	ILE	A	628	3.146	34.065	7.805	1.00	59.16	C
ATOM	780	CD1	ILE	A	628	1.926	34.642	8.530	1.00	58.40	C
ATOM	781	C	ILE	A	628	6.480	32.456	8.894	1.00	61.87	C
ATOM	782	O	ILE	A	628	6.488	31.224	9.012	1.00	61.25	O
ATOM	783	N	ILE	A	629	7.322	33.256	9.557	1.00	64.50	N
ATOM	784	CA	ILE	A	629	8.294	32.752	10.529	1.00	66.21	C
ATOM	785	CB	ILE	A	629	9.670	32.594	9.906	1.00	64.27	C
ATOM	786	CG2	ILE	A	629	10.575	31.858	10.871	1.00	62.84	C
ATOM	787	CG1	ILE	A	629	9.538	31.824	8.593	1.00	64.22	C
ATOM	788	CD1	ILE	A	629	10.834	31.451	7.949	1.00	65.97	C
ATOM	789	C	ILE	A	629	8.403	33.633	11.783	1.00	69.29	C
ATOM	790	O	ILE	A	629	8.636	34.840	11.716	1.00	69.32	O
ATOM	791	N	ASN	A	630	8.233	32.982	12.929	1.00	73.87	N
ATOM	792	CA	ASN	A	630	8.243	33.594	14.262	1.00	77.51	C
ATOM	793	CB	ASN	A	630	7.174	32.890	15.084	1.00	79.26	C
ATOM	794	CG	ASN	A	630	6.857	31.513	14.530	1.00	81.12	C
ATOM	795	OD1	ASN	A	630	6.259	31.392	13.464	1.00	80.98	O
ATOM	796	ND2	ASN	A	630	7.291	30.467	15.235	1.00	81.86	N
ATOM	797	C	ASN	A	630	9.593	33.477	14.972	1.00	79.33	C
ATOM	798	O	ASN	A	630	10.639	33.424	14.320	1.00	79.88	O



ATOM	880	CD2	TYR	A	640	18.938	34.503	15.403	1.00	73.13	C
ATOM	881	CE2	TYR	A	640	18.676	35.488	16.342	1.00	73.23	C
ATOM	882	CZ	TYR	A	640	17.389	35.984	16.491	1.00	73.89	C
ATOM	883	OH	TYR	A	640	17.154	36.994	17.394	1.00	75.08	O
ATOM	884	C	TYR	A	640	19.318	34.701	12.113	1.00	75.43	C
ATOM	885	O	TYR	A	640	19.046	35.884	12.321	1.00	75.02	O
ATOM	886	N	ASP	A	641	20.544	34.257	11.880	1.00	75.46	N
ATOM	887	CA	ASP	A	641	21.689	35.146	11.830	1.00	75.75	C
ATOM	888	CB	ASP	A	641	22.955	34.323	11.610	1.00	78.65	C
ATOM	889	CG	ASP	A	641	22.875	33.478	10.369	1.00	81.73	C
ATOM	890	OD1	ASP	A	641	21.798	32.867	10.152	1.00	82.69	O
ATOM	891	OD2	ASP	A	641	23.886	33.431	9.626	1.00	82.69	O
ATOM	892	C	ASP	A	641	21.468	36.120	10.686	1.00	73.93	C
ATOM	893	O	ASP	A	641	22.159	37.136	10.569	1.00	73.31	O
ATOM	894	N	GLN	A	642	20.493	35.787	9.844	1.00	73.01	N
ATOM	895	CA	GLN	A	642	20.130	36.620	8.704	1.00	72.29	C
ATOM	896	CB	GLN	A	642	20.221	35.819	7.397	1.00	73.06	C
ATOM	897	CG	GLN	A	642	19.405	34.549	7.347	1.00	73.57	C
ATOM	898	CD	GLN	A	642	20.250	33.346	6.960	1.00	74.07	C
ATOM	899	OE1	GLN	A	642	20.693	32.591	7.813	1.00	76.16	O
ATOM	900	NE2	GLN	A	642	20.481	33.170	5.665	1.00	73.49	N
ATOM	901	C	GLN	A	642	18.723	37.166	8.908	1.00	69.89	C
ATOM	902	O	GLN	A	642	18.427	38.302	8.538	1.00	70.05	O
ATOM	903	N	CYS	A	643	17.859	36.355	9.510	1.00	68.20	N
ATOM	904	CA	CYS	A	643	16.493	36.782	9.798	1.00	66.80	C
ATOM	905	CB	CYS	A	643	15.691	35.642	10.400	1.00	64.52	C
ATOM	906	SG	CYS	A	643	15.620	34.242	9.324	1.00	62.12	S
ATOM	907	C	CYS	A	643	16.538	37.914	10.800	1.00	66.28	C
ATOM	908	O	CYS	A	643	15.609	38.716	10.888	1.00	64.96	O
ATOM	909	N	LYS	A	644	17.627	37.957	11.561	1.00	66.18	N
ATOM	910	CA	LYS	A	644	17.812	38.988	12.565	1.00	66.37	C
ATOM	911	CB	LYS	A	644	18.959	38.608	13.509	1.00	68.66	C
ATOM	912	CG	LYS	A	644	19.070	39.500	14.740	1.00	72.51	C
ATOM	913	CD	LYS	A	644	20.089	38.962	15.740	1.00	75.50	C
ATOM	914	CE	LYS	A	644	20.137	39.791	17.025	1.00	77.12	C
ATOM	915	NZ	LYS	A	644	21.143	39.250	17.988	1.00	78.05	N
ATOM	916	C	LYS	A	644	18.092	40.318	11.866	1.00	64.80	C
ATOM	917	O	LYS	A	644	17.910	41.391	12.446	1.00	65.34	O
ATOM	918	N	HIS	A	645	18.510	40.230	10.606	1.00	63.00	N
ATOM	919	CA	HIS	A	645	18.802	41.405	9.801	1.00	59.77	C
ATOM	920	CB	HIS	A	645	19.743	41.037	8.659	1.00	59.92	C
ATOM	921	CG	HIS	A	645	21.140	40.753	9.109	1.00	59.70	C
ATOM	922	CD2	HIS	A	645	21.852	39.602	9.132	1.00	58.68	C
ATOM	923	ND1	HIS	A	645	21.960	41.728	9.638	1.00	58.42	N
ATOM	924	CE1	HIS	A	645	23.117	41.185	9.966	1.00	59.06	C
ATOM	925	NE2	HIS	A	645	23.080	39.898	9.671	1.00	59.02	N
ATOM	926	C	HIS	A	645	17.498	41.929	9.260	1.00	58.18	C
ATOM	927	O	HIS	A	645	17.203	43.114	9.396	1.00	57.96	O
ATOM	928	N	MET	A	646	16.713	41.037	8.659	1.00	57.42	N
ATOM	929	CA	MET	A	646	15.404	41.402	8.113	1.00	56.10	C
ATOM	930	CB	MET	A	646	14.743	40.195	7.425	1.00	56.15	C
ATOM	931	CG	MET	A	646	15.430	39.717	6.142	1.00	57.62	C
ATOM	932	SD	MET	A	646	15.933	37.957	6.139	1.00	59.85	S
ATOM	933	CE	MET	A	646	14.564	37.207	5.554	1.00	58.77	C
ATOM	934	C	MET	A	646	14.505	41.896	9.240	1.00	54.90	C
ATOM	935	O	MET	A	646	13.758	42.854	9.068	1.00	54.02	O
ATOM	936	N	LEU	A	647	14.588	41.232	10.392	1.00	54.19	N
ATOM	937	CA	LEU	A	647	13.784	41.589	11.557	1.00	51.72	C
ATOM	938	CB	LEU	A	647	14.165	40.699	12.731	1.00	50.92	C
ATOM	939	CG	LEU	A	647	13.183	39.576	13.077	1.00	51.35	C
ATOM	940	CD1	LEU	A	647	12.193	39.278	11.918	1.00	49.77	C
ATOM	941	CD2	LEU	A	647	14.018	38.359	13.488	1.00	49.26	C
ATOM	942	C	LEU	A	647	14.015	43.041	11.893	1.00	51.19	C
ATOM	943	O	LEU	A	647	13.101	43.763	12.291	1.00	51.34	O
ATOM	944	N	TYR	A	648	15.255	43.472	11.724	1.00	49.86	N
ATOM	945	CA	TYR	A	648	15.596	44.855	12.008	1.00	47.81	C
ATOM	946	CB	TYR	A	648	17.015	45.144	11.531	1.00	44.66	C
ATOM	947	CG	TYR	A	648	17.354	46.618	11.497	1.00	42.49	C
ATOM	948	CD1	TYR	A	648	17.469	47.365	12.671	1.00	40.92	C
ATOM	949	CE1	TYR	A	648	17.808	48.720	12.633	1.00	40.43	C
ATOM	950	CD2	TYR	A	648	17.578	47.264	10.285	1.00	41.74	C
ATOM	951	CE2	TYR	A	648	17.913	48.608	10.238	1.00	41.65	C
ATOM	952	CZ	TYR	A	648	18.031	49.328	11.407	1.00	41.29	C
ATOM	953	OH	TYR	A	648	18.393	50.648	11.322	1.00	42.63	O
ATOM	954	C	TYR	A	648	14.620	45.808	11.316	1.00	47.45	C
ATOM	955	O	TYR	A	648	14.071	46.718	11.940	1.00	46.64	O
ATOM	956	N	VAL	A	649	14.413	45.578	10.023	1.00	46.91	N
ATOM	957	CA	VAL	A	649	13.535	46.411	9.216	1.00	47.52	C
ATOM	958	CB	VAL	A	649	13.394	45.861	7.801	1.00	48.32	C
ATOM	959	CG1	VAL	A	649	12.596	46.840	6.924	1.00	47.29	C
ATOM	960	CG2	VAL	A	649	14.772	45.585	7.237	1.00	47.74	C

ATOM	961	C	VAL	A	649	12.155	46.528	9.810	1.00	48.22	C
ATOM	962	O	VAL	A	649	11.720	47.630	10.119	1.00	48.77	O
ATOM	963	N	SER	A	650	11.468	45.397	9.964	1.00	49.23	N
ATOM	964	CA	SER	A	650	10.114	45.383	10.523	1.00	50.65	C
ATOM	965	CB	SER	A	650	9.585	43.941	10.637	1.00	51.24	C
ATOM	966	OG	SER	A	650	10.393	43.161	11.500	1.00	53.81	O
ATOM	967	C	SER	A	650	10.014	46.056	11.890	1.00	50.66	C
ATOM	968	O	SER	A	650	9.070	46.803	12.156	1.00	49.51	O
ATOM	969	N	SER	A	651	10.991	45.787	12.753	1.00	50.55	N
ATOM	970	CA	SER	A	651	11.017	46.361	14.095	1.00	51.09	C
ATOM	971	CB	SER	A	651	12.170	45.770	14.899	1.00	51.47	C
ATOM	972	OG	SER	A	651	13.335	45.701	14.098	1.00	55.27	O
ATOM	973	C	SER	A	651	11.163	47.873	14.018	1.00	51.11	C
ATOM	974	O	SER	A	651	10.522	48.610	14.763	1.00	52.23	O
ATOM	975	N	GLU	A	652	12.004	48.341	13.111	1.00	51.58	N
ATOM	976	CA	GLU	A	652	12.206	49.771	12.954	1.00	52.96	C
ATOM	977	CB	GLU	A	652	13.461	50.009	12.101	1.00	53.40	C
ATOM	978	CG	GLU	A	652	14.158	51.358	12.295	1.00	52.80	C
ATOM	979	CD	GLU	A	652	14.660	51.550	13.709	1.00	53.12	C
ATOM	980	OE1	GLU	A	652	14.836	50.524	14.405	1.00	52.90	O
ATOM	981	OE2	GLU	A	652	14.884	52.713	14.116	1.00	51.83	O
ATOM	982	C	GLU	A	652	10.964	50.330	12.254	1.00	54.01	C
ATOM	983	O	GLU	A	652	10.541	51.470	12.483	1.00	54.79	O
ATOM	984	N	LEU	A	653	10.366	49.503	11.408	1.00	55.58	N
ATOM	985	CA	LEU	A	653	9.184	49.905	10.661	1.00	57.21	C
ATOM	986	CB	LEU	A	653	8.998	48.956	9.470	1.00	53.73	C
ATOM	987	CG	LEU	A	653	8.452	49.539	8.174	1.00	51.55	C
ATOM	988	CD1	LEU	A	653	9.167	50.851	7.831	1.00	51.81	C
ATOM	989	CD2	LEU	A	653	8.616	48.497	7.062	1.00	49.87	C
ATOM	990	C	LEU	A	653	7.981	49.877	11.608	1.00	58.50	C
ATOM	991	O	LEU	A	653	6.856	50.233	11.243	1.00	60.00	O
ATOM	992	N	HIS	A	654	8.256	49.485	12.847	1.00	58.33	N
ATOM	993	CA	HIS	A	654	7.244	49.384	13.890	1.00	57.70	C
ATOM	994	CB	HIS	A	654	7.328	48.002	14.553	1.00	57.91	C
ATOM	995	CG	HIS	A	654	6.462	47.854	15.761	1.00	58.06	C
ATOM	996	CD2	HIS	A	654	6.758	47.914	17.083	1.00	58.87	C
ATOM	997	ND1	HIS	A	654	5.099	47.664	15.686	1.00	58.93	N
ATOM	998	CE1	HIS	A	654	4.593	47.617	16.908	1.00	59.08	C
ATOM	999	NE2	HIS	A	654	5.579	47.766	17.769	1.00	59.13	N
ATOM	1000	C	HIS	A	654	7.509	50.466	14.919	1.00	56.80	C
ATOM	1001	O	HIS	A	654	6.583	51.120	15.401	1.00	55.50	O
ATOM	1002	N	ARG	A	655	8.784	50.635	15.256	1.00	56.90	N
ATOM	1003	CA	ARG	A	655	9.204	51.650	16.210	1.00	58.18	C
ATOM	1004	CB	ARG	A	655	10.726	51.625	16.385	1.00	58.72	C
ATOM	1005	CG	ARG	A	655	11.267	52.736	17.274	1.00	57.26	C
ATOM	1006	CD	ARG	A	655	12.768	52.670	17.303	1.00	57.06	C
ATOM	1007	NE	ARG	A	655	13.384	53.342	16.164	1.00	58.45	N
ATOM	1008	CZ	ARG	A	655	13.349	54.656	15.942	1.00	60.38	C
ATOM	1009	NH1	ARG	A	655	12.712	55.464	16.780	1.00	59.14	N
ATOM	1010	NH2	ARG	A	655	13.992	55.173	14.899	1.00	58.16	N
ATOM	1011	C	ARG	A	655	8.809	53.043	15.720	1.00	58.84	C
ATOM	1012	O	ARG	A	655	8.391	53.896	16.506	1.00	59.48	O
ATOM	1013	N	LEU	A	656	8.946	53.268	14.417	1.00	58.42	N
ATOM	1014	CA	LEU	A	656	8.636	54.566	13.830	1.00	58.31	C
ATOM	1015	CB	LEU	A	656	9.574	54.828	12.643	1.00	59.21	C
ATOM	1016	CG	LEU	A	656	10.243	56.207	12.513	1.00	58.41	C
ATOM	1017	CD1	LEU	A	656	10.743	56.697	13.857	1.00	57.20	C
ATOM	1018	CD2	LEU	A	656	11.401	56.108	11.549	1.00	58.13	C
ATOM	1019	C	LEU	A	656	7.185	54.639	13.382	1.00	58.15	C
ATOM	1020	O	LEU	A	656	6.683	55.714	13.056	1.00	56.91	O
ATOM	1021	N	GLN	A	657	6.525	53.483	13.382	1.00	58.20	N
ATOM	1022	CA	GLN	A	657	5.125	53.366	12.985	1.00	58.07	C
ATOM	1023	CB	GLN	A	657	4.212	53.969	14.049	1.00	59.63	C
ATOM	1024	CG	GLN	A	657	4.148	53.161	15.325	1.00	63.04	C
ATOM	1025	CD	GLN	A	657	2.815	53.310	16.047	1.00	66.34	C
ATOM	1026	OE1	GLN	A	657	2.389	54.424	16.371	1.00	68.74	O
ATOM	1027	NE2	GLN	A	657	2.151	52.184	16.307	1.00	66.39	N
ATOM	1028	C	GLN	A	657	4.845	54.045	11.664	1.00	56.24	C
ATOM	1029	O	GLN	A	657	3.973	54.906	11.587	1.00	56.39	O
ATOM	1030	N	VAL	A	658	5.588	53.653	10.632	1.00	53.53	N
ATOM	1031	CA	VAL	A	658	5.440	54.222	9.294	1.00	49.80	C
ATOM	1032	CB	VAL	A	658	6.506	53.641	8.343	1.00	49.06	C
ATOM	1033	CG1	VAL	A	658	6.385	54.251	6.942	1.00	49.12	C
ATOM	1034	CG2	VAL	A	658	7.871	53.882	8.932	1.00	48.69	C
ATOM	1035	C	VAL	A	658	4.066	53.923	8.736	1.00	47.47	C
ATOM	1036	O	VAL	A	658	3.486	52.874	9.018	1.00	48.37	O
ATOM	1037	N	SER	A	659	3.536	54.857	7.957	1.00	44.90	N
ATOM	1038	CA	SER	A	659	2.233	54.662	7.221	1.00	41.14	C
ATOM	1039	CB	SER	A	659	1.498	55.993	6.199	1.00	38.28	C
ATOM	1040	OG	SER	A	659	2.068	56.781	5.946	1.00	44.11	O
ATOM	1041	C	SER	A	659	2.371	54.020				C

ATOM	1042	O	SER	A	659	3.474	53.878	5.415	1.00	45.44	O
ATOM	1043	N	TYR	A	660	1.245	53.636	5.354	1.00	43.08	N
ATOM	1044	CA	TYR	A	660	1.259	52.996	4.043	1.00	42.59	C
ATOM	1045	CB	TYR	A	660	-0.132	52.480	3.694	1.00	40.73	C
ATOM	1046	CG	TYR	A	660	-0.179	51.708	2.397	1.00	39.79	C
ATOM	1047	CD1	TYR	A	660	0.551	50.522	2.236	1.00	39.97	C
ATOM	1048	CE1	TYR	A	660	0.519	49.819	1.029	1.00	39.11	C
ATOM	1049	CD2	TYR	A	660	-0.940	52.164	1.321	1.00	38.28	C
ATOM	1050	CE2	TYR	A	660	-0.976	51.470	0.117	1.00	36.89	C
ATOM	1051	CZ	TYR	A	660	-0.255	50.301	-0.020	1.00	37.99	C
ATOM	1052	OH	TYR	A	660	-0.347	49.584	-1.183	1.00	40.38	O
ATOM	1053	C	TYR	A	660	1.698	54.002	2.998	1.00	43.53	C
ATOM	1054	O	TYR	A	660	2.381	53.682	2.023	1.00	40.82	O
ATOM	1055	N	GLU	A	661	1.281	55.235	3.216	1.00	45.17	N
ATOM	1056	CA	GLU	A	661	1.621	56.316	2.319	1.00	47.43	C
ATOM	1057	CB	GLU	A	661	0.852	57.571	2.746	1.00	51.28	C
ATOM	1058	CG	GLU	A	661	0.492	58.562	1.631	1.00	54.68	C
ATOM	1059	CD	GLU	A	661	-1.004	58.560	1.301	1.00	56.32	C
ATOM	1060	OE1	GLU	A	661	-1.820	58.704	2.231	1.00	58.17	O
ATOM	1061	OE2	GLU	A	661	-1.379	58.416	0.123	1.00	57.76	O
ATOM	1062	C	GLU	A	661	3.136	56.575	2.382	1.00	46.75	C
ATOM	1063	O	GLU	A	661	3.822	56.651	1.355	1.00	46.32	O
ATOM	1064	N	GLU	A	662	3.652	56.723	3.598	1.00	45.63	N
ATOM	1065	CA	GLU	A	662	5.074	56.988	3.771	1.00	45.45	C
ATOM	1066	CB	GLU	A	662	5.412	57.222	5.256	1.00	44.64	C
ATOM	1067	CG	GLU	A	662	4.627	58.363	5.915	1.00	44.59	C
ATOM	1068	CD	GLU	A	662	4.857	58.467	7.419	1.00	46.79	C
ATOM	1069	OE1	GLU	A	662	5.028	57.414	8.079	1.00	46.01	O
ATOM	1070	OE2	GLU	A	662	4.854	59.609	7.952	1.00	47.97	O
ATOM	1071	C	GLU	A	662	5.866	55.805	3.239	1.00	44.16	C
ATOM	1072	O	GLU	A	662	6.868	55.962	2.542	1.00	45.27	O
ATOM	1073	N	TYR	A	663	5.386	54.614	3.561	1.00	43.82	N
ATOM	1074	CA	TYR	A	663	6.027	53.394	3.128	1.00	41.69	C
ATOM	1075	CB	TYR	A	663	5.221	52.199	3.614	1.00	39.69	C
ATOM	1076	CG	TYR	A	663	5.533	50.923	2.882	1.00	40.59	C
ATOM	1077	CD1	TYR	A	663	6.774	50.297	3.010	1.00	42.11	C
ATOM	1078	CE1	TYR	A	663	7.082	49.131	2.280	1.00	43.17	C
ATOM	1079	CD2	TYR	A	663	4.601	50.361	2.012	1.00	41.89	C
ATOM	1080	CE2	TYR	A	663	4.889	49.206	1.280	1.00	43.67	C
ATOM	1081	CZ	TYR	A	663	6.130	48.593	1.410	1.00	44.34	C
ATOM	1082	OH	TYR	A	663	6.408	47.455	0.661	1.00	46.31	O
ATOM	1083	C	TYR	A	663	6.162	53.365	1.615	1.00	41.38	C
ATOM	1084	O	TYR	A	663	7.240	53.094	1.104	1.00	44.00	O
ATOM	1085	N	LEU	A	664	5.079	53.660	0.899	1.00	40.00	N
ATOM	1086	CA	LEU	A	664	5.094	53.634	-0.562	1.00	37.88	C
ATOM	1087	CB	LEU	A	664	3.685	53.905	-1.103	1.00	37.12	C
ATOM	1088	CG	LEU	A	664	2.711	52.724	-1.027	1.00	37.53	C
ATOM	1089	CD1	LEU	A	664	1.373	53.176	-1.611	1.00	37.45	C
ATOM	1090	CD2	LEU	A	664	3.260	51.495	-1.786	1.00	35.07	C
ATOM	1091	C	LEU	A	664	6.101	54.615	-1.175	1.00	37.10	C
ATOM	1092	O	LEU	A	664	6.612	54.402	-2.285	1.00	35.66	O
ATOM	1093	N	CYS	A	665	6.393	55.681	-0.442	1.00	35.22	N
ATOM	1094	CA	CYS	A	665	7.338	56.679	-0.915	1.00	37.04	C
ATOM	1095	CB	CYS	A	665	7.020	58.047	-0.299	1.00	37.41	C
ATOM	1096	SG	CYS	A	665	5.554	58.846	-1.006	1.00	40.10	S
ATOM	1097	C	CYS	A	665	8.772	56.275	-0.589	1.00	38.08	C
ATOM	1098	O	CYS	A	665	9.692	56.491	-1.387	1.00	37.65	O
ATOM	1099	N	MET	A	666	8.948	55.693	0.592	1.00	37.80	N
ATOM	1100	CA	MET	A	666	10.240	55.206	1.037	1.00	37.89	C
ATOM	1101	CB	MET	A	666	10.137	54.654	2.463	1.00	39.50	C
ATOM	1102	CG	MET	A	666	9.831	55.691	3.517	1.00	41.45	C
ATOM	1103	SD	MET	A	666	9.712	54.903	5.105	1.00	44.06	S
ATOM	1104	CE	MET	A	666	11.484	54.731	5.457	1.00	44.38	C
ATOM	1105	C	MET	A	666	10.738	54.087	0.116	1.00	38.44	C
ATOM	1106	O	MET	A	666	11.933	53.997	-0.171	1.00	39.89	O
ATOM	1107	N	LYS	A	667	9.821	53.239	-0.350	1.00	36.26	N
ATOM	1108	CA	LYS	A	667	10.199	52.127	-1.211	1.00	35.46	C
ATOM	1109	CB	LYS	A	667	9.053	51.116	-1.322	1.00	35.39	C
ATOM	1110	CG	LYS	A	667	9.457	49.758	-1.876	1.00	33.89	C
ATOM	1111	CD	LYS	A	667	8.394	48.703	-1.545	1.00	34.45	C
ATOM	1112	CE	LYS	A	667	7.002	49.059	-2.109	1.00	35.03	C
ATOM	1113	NZ	LYS	A	667	7.042	49.199	-3.603	1.00	35.14	N
ATOM	1114	C	LYS	A	667	10.580	52.639	-2.582	1.00	34.54	C
ATOM	1115	O	LYS	A	667	11.343	51.998	-3.293	1.00	34.12	O
ATOM	1116	N	THR	A	668	10.066	53.807	-2.951	1.00	34.65	N
ATOM	1117	CA	THR	A	668	10.384	54.343	-4.266	1.00	36.42	C
ATOM	1118	CB	THR	A	668	9.336	55.412	-4.743	1.00	34.99	C
ATOM	1119	OG1	THR	A	668	8.124	54.774	-5.157	1.00	32.53	O
ATOM	1120	CG2	THR	A	668	9.857	56.172	-5.924	1.00	32.92	C
ATOM	1121	C	THR	A	668	11.772	54.977	-4.205	1.00	37.15	C
ATOM	1122	O	THR	A	668	12.601	54.757	-5.081	1.00	39.05	O

ATOM	1123	N	LEU	A	669	12.012	55.771	-3.169	1.00	38.42	N
ATOM	1124	CA	LEU	A	669	13.289	56.430	-2.983	1.00	39.07	C
ATOM	1125	CB	LEU	A	669	13.257	57.261	-1.704	1.00	35.34	C
ATOM	1126	CG	LEU	A	669	12.440	58.556	-1.774	1.00	33.99	C
ATOM	1127	CD1	LEU	A	669	12.520	59.237	-0.426	1.00	32.37	C
ATOM	1128	CD2	LEU	A	669	12.966	59.498	-2.864	1.00	29.80	C
ATOM	1129	C	LEU	A	669	14.420	55.401	-2.927	1.00	42.20	C
ATOM	1130	O	LEU	A	669	15.590	55.725	-3.136	1.00	43.83	O
ATOM	1131	N	LEU	A	670	14.069	54.157	-2.636	1.00	44.48	N
ATOM	1132	CA	LEU	A	670	15.069	53.111	-2.596	1.00	46.88	C
ATOM	1133	CB	LEU	A	670	14.539	51.876	-1.885	1.00	45.00	C
ATOM	1134	CG	LEU	A	670	14.451	51.950	-0.367	1.00	43.33	C
ATOM	1135	CD1	LEU	A	670	13.806	50.676	0.164	1.00	44.23	C
ATOM	1136	CD2	LEU	A	670	15.843	52.114	0.211	1.00	41.37	C
ATOM	1137	C	LEU	A	670	15.473	52.738	-4.010	1.00	49.44	C
ATOM	1138	O	LEU	A	670	16.655	52.578	-4.296	1.00	52.76	O
ATOM	1139	N	LEU	A	671	14.492	52.585	-4.893	1.00	51.63	N
ATOM	1140	CA	LEU	A	671	14.754	52.241	-6.289	1.00	53.74	C
ATOM	1141	CB	LEU	A	671	13.428	52.173	-7.055	1.00	53.98	C
ATOM	1142	CG	LEU	A	671	13.394	51.837	-8.559	1.00	55.20	C
ATOM	1143	CD1	LEU	A	671	13.602	53.103	-9.350	1.00	55.57	C
ATOM	1144	CD2	LEU	A	671	14.442	50.772	-8.933	1.00	55.85	C
ATOM	1145	C	LEU	A	671	15.670	53.291	-6.917	1.00	55.81	C
ATOM	1146	O	LEU	A	671	16.531	52.986	-7.741	1.00	54.57	O
ATOM	1147	N	LEU	A	672	15.482	54.534	-6.502	1.00	58.80	N
ATOM	1148	CA	LEU	A	672	16.268	55.641	-7.022	1.00	62.80	C
ATOM	1149	CB	LEU	A	672	15.334	56.799	-7.371	1.00	61.85	C
ATOM	1150	CG	LEU	A	672	14.134	56.447	-8.259	1.00	60.89	C
ATOM	1151	CD1	LEU	A	672	13.084	57.539	-8.128	1.00	61.15	C
ATOM	1152	CD2	LEU	A	672	14.582	56.266	-9.706	1.00	59.60	C
ATOM	1153	C	LEU	A	672	17.268	56.092	-5.970	1.00	65.84	C
ATOM	1154	O	LEU	A	672	17.505	57.281	-5.798	1.00	66.23	O
ATOM	1155	N	SER	A	673	17.860	55.145	-5.260	1.00	69.11	N
ATOM	1156	CA	SER	A	673	18.800	55.511	-4.221	1.00	71.93	C
ATOM	1157	CB	SER	A	673	18.906	54.382	-3.210	1.00	71.47	C
ATOM	1158	OG	SER	A	673	18.853	54.877	-1.885	1.00	71.88	O
ATOM	1159	C	SER	A	673	20.170	55.845	-4.782	1.00	75.36	C
ATOM	1160	O	SER	A	673	20.369	56.932	-5.349	1.00	76.01	O
ATOM	1161	N	SER	A	674	21.108	54.911	-4.651	1.00	78.75	N
ATOM	1162	CA	SER	A	674	22.460	55.149	-5.134	1.00	81.66	C
ATOM	1163	CB	SER	A	674	23.442	54.046	-4.651	1.00	82.06	C
ATOM	1164	OG	SER	A	674	23.730	54.142	-3.253	1.00	80.07	O
ATOM	1165	C	SER	A	674	22.578	55.331	-6.651	1.00	83.67	C
ATOM	1166	O	SER	A	674	21.590	55.440	-7.385	1.00	83.37	O
ATOM	1167	N	VAL	A	675	23.832	55.388	-7.086	1.00	85.82	N
ATOM	1168	CA	VAL	A	675	24.209	55.616	-8.471	1.00	87.39	C
ATOM	1169	CB	VAL	A	675	23.966	57.099	-8.851	1.00	86.61	C
ATOM	1170	CG1	VAL	A	675	24.995	57.586	-9.881	1.00	86.91	C
ATOM	1171	CG2	VAL	A	675	22.560	57.257	-9.382	1.00	86.19	C
ATOM	1172	C	VAL	A	675	25.698	55.337	-8.513	1.00	89.13	C
ATOM	1173	O	VAL	A	675	26.406	55.602	-7.534	1.00	88.61	O
ATOM	1174	N	PRO	A	676	26.191	54.792	-9.638	1.00	90.50	N
ATOM	1175	CD	PRO	A	676	25.444	54.551	-10.891	1.00	91.19	C
ATOM	1176	CA	PRO	A	676	27.612	54.473	-9.809	1.00	91.78	C
ATOM	1177	CB	PRO	A	676	27.767	54.423	-11.326	1.00	91.81	C
ATOM	1178	CG	PRO	A	676	26.454	53.806	-11.753	1.00	91.79	C
ATOM	1179	C	PRO	A	676	28.495	55.530	-9.161	1.00	91.76	C
ATOM	1180	O	PRO	A	676	28.940	55.365	-8.028	1.00	92.62	O
ATOM	1181	N	LYS	A	677	28.743	56.615	-9.890	1.00	91.42	N
ATOM	1182	CA	LYS	A	677	29.550	57.725	-9.386	1.00	90.59	C
ATOM	1183	CB	LYS	A	677	30.803	57.213	-8.658	1.00	89.47	C
ATOM	1184	CG	LYS	A	677	31.020	57.863	-7.291	1.00	88.66	C
ATOM	1185	CD	LYS	A	677	29.720	57.935	-6.487	1.00	88.80	C
ATOM	1186	CE	LYS	A	677	29.029	59.294	-6.622	1.00	88.91	C
ATOM	1187	NZ	LYS	A	677	27.550	59.266	-6.374	1.00	88.10	N
ATOM	1188	C	LYS	A	677	29.942	58.657	-10.527	1.00	90.29	C
ATOM	1189	O	LYS	A	677	30.165	59.849	-10.322	1.00	90.63	O
ATOM	1190	N	ASP	A	678	30.009	58.110	-11.736	1.00	89.62	N
ATOM	1191	CA	ASP	A	678	30.357	58.893	-12.920	1.00	88.89	C
ATOM	1192	CB	ASP	A	678	31.063	58.000	-13.959	1.00	89.19	C
ATOM	1193	CG	ASP	A	678	32.011	58.778	-14.874	1.00	88.51	C
ATOM	1194	OD1	ASP	A	678	31.553	59.707	-15.579	1.00	88.03	O
ATOM	1195	OD2	ASP	A	678	33.217	58.449	-14.889	1.00	87.03	O
ATOM	1196	C	ASP	A	678	29.048	59.442	-13.497	1.00	87.61	C
ATOM	1197	O	ASP	A	678	28.974	59.827	-14.666	1.00	87.58	O
ATOM	1198	N	GLY	A	679	28.025	59.489	-12.648	1.00	86.16	N
ATOM	1199	CA	GLY	A	679	26.724	59.967	-13.071	1.00	84.02	C
ATOM	1200	C	GLY	A	679	26.069	59.059	-14.103	1.00	82.62	C
ATOM	1201	O	GLY	A	679	26.669	58.729	-15.130	1.00	83.22	O
ATOM	1202	N	LEU	A	680	24.839	58.637	-13.828	1.00	80.01	N
ATOM	1203	CA	LEU	A	680	24.105	57.788	-14.760	1.00	76.98	C

ATOM	1204	CB	LEU	A	680	22.678	57.548	-14.239	1.00	76.06	C
ATOM	1205	CG	LEU	A	680	22.495	56.910	-12.855	1.00	74.98	C
ATOM	1206	CD1	LEU	A	680	21.079	57.146	-12.341	1.00	73.06	C
ATOM	1207	CD2	LEU	A	680	22.803	55.424	-12.946	1.00	73.24	C
ATOM	1208	C	LEU	A	680	24.048	58.523	-16.107	1.00	75.06	C
ATOM	1209	O	LEU	A	680	24.229	59.744	-16.167	1.00	74.11	O
ATOM	1210	N	LYS	A	681	23.815	57.779	-17.184	1.00	72.73	N
ATOM	1211	CA	LYS	A	681	23.715	58.390	-18.505	1.00	70.21	C
ATOM	1212	CB	LYS	A	681	23.334	57.347	-19.557	1.00	69.31	C
ATOM	1213	CG	LYS	A	681	24.518	56.705	-20.250	1.00	68.29	C
ATOM	1214	CD	LYS	A	681	25.341	55.843	-19.300	1.00	67.55	C
ATOM	1215	CE	LYS	A	681	26.494	55.160	-20.036	1.00	65.59	C
ATOM	1216	NZ	LYS	A	681	26.039	54.391	-21.236	1.00	61.64	N
ATOM	1217	C	LYS	A	681	22.675	59.506	-18.506	1.00	69.59	C
ATOM	1218	O	LYS	A	681	22.813	60.493	-19.223	1.00	70.85	O
ATOM	1219	N	SER	A	682	21.639	59.346	-17.688	1.00	68.16	N
ATOM	1220	CA	SER	A	682	20.561	60.325	-17.594	1.00	65.66	C
ATOM	1221	CB	SER	A	682	19.230	59.641	-17.871	1.00	65.37	C
ATOM	1222	OG	SER	A	682	19.333	58.829	-19.020	1.00	64.33	O
ATOM	1223	C	SER	A	682	20.514	60.931	-16.203	1.00	64.67	C
ATOM	1224	O	SER	A	682	19.456	60.939	-15.587	1.00	63.62	O
ATOM	1225	N	GLN	A	683	21.644	61.440	-15.714	1.00	64.38	N
ATOM	1226	CA	GLN	A	683	21.700	62.018	-14.370	1.00	65.18	C
ATOM	1227	CB	GLN	A	683	23.121	62.502	-14.061	1.00	64.99	C
ATOM	1228	CG	GLN	A	683	23.280	63.042	-12.656	1.00	65.80	C
ATOM	1229	CD	GLN	A	683	23.132	61.958	-11.625	1.00	66.15	C
ATOM	1230	OE1	GLN	A	683	22.902	62.226	-10.448	1.00	66.81	O
ATOM	1231	NE2	GLN	A	683	23.272	60.713	-12.062	1.00	67.81	N
ATOM	1232	C	GLN	A	683	20.697	63.163	-14.203	1.00	65.30	C
ATOM	1233	O	GLN	A	683	20.204	63.432	-13.104	1.00	64.40	O
ATOM	1234	N	GLU	A	684	20.391	63.824	-15.313	1.00	65.93	N
ATOM	1235	CA	GLU	A	684	19.441	64.932	-15.314	1.00	66.98	C
ATOM	1236	CB	GLU	A	684	19.455	65.635	-16.674	1.00	68.74	C
ATOM	1237	CG	GLU	A	684	20.576	65.189	-17.591	1.00	70.85	C
ATOM	1238	CD	GLU	A	684	20.432	63.745	-18.010	1.00	72.48	C
ATOM	1239	OE1	GLU	A	684	21.393	63.199	-18.589	1.00	72.54	O
ATOM	1240	OE2	GLU	A	684	19.351	63.161	-17.763	1.00	74.49	O
ATOM	1241	C	GLU	A	684	18.028	64.425	-15.017	1.00	66.33	C
ATOM	1242	O	GLU	A	684	17.307	65.001	-14.201	1.00	65.98	O
ATOM	1243	N	LEU	A	685	17.641	63.350	-15.695	1.00	64.94	N
ATOM	1244	CA	LEU	A	685	16.330	62.735	-15.513	1.00	64.26	C
ATOM	1245	CB	LEU	A	685	16.139	61.652	-16.583	1.00	64.30	C
ATOM	1246	CG	LEU	A	685	14.937	61.786	-17.514	1.00	64.98	C
ATOM	1247	CD1	LEU	A	685	15.334	61.277	-18.894	1.00	65.94	C
ATOM	1248	CD2	LEU	A	685	13.728	61.041	-16.941	1.00	65.67	C
ATOM	1249	C	LEU	A	685	16.186	62.126	-14.103	1.00	63.99	C
ATOM	1250	O	LEU	A	685	15.129	62.236	-13.466	1.00	64.87	O
ATOM	1251	N	PHE	A	686	17.265	61.506	-13.623	1.00	62.00	N
ATOM	1252	CA	PHE	A	686	17.288	60.862	-12.313	1.00	58.97	C
ATOM	1253	CB	PHE	A	686	18.649	60.196	-12.059	1.00	56.27	C
ATOM	1254	CG	PHE	A	686	18.642	59.226	-10.909	1.00	52.68	C
ATOM	1255	CD1	PHE	A	686	17.973	58.010	-11.018	1.00	52.02	C
ATOM	1256	CD2	PHE	A	686	19.268	59.536	-9.712	1.00	50.53	C
ATOM	1257	CE1	PHE	A	686	17.928	57.118	-9.942	1.00	52.59	C
ATOM	1258	CE2	PHE	A	686	19.227	58.648	-8.630	1.00	50.89	C
ATOM	1259	CZ	PHE	A	686	18.554	57.437	-8.747	1.00	50.63	C
ATOM	1260	C	PHE	A	686	16.983	61.846	-11.189	1.00	58.51	C
ATOM	1261	O	PHE	A	686	15.989	61.694	-10.487	1.00	58.68	O
ATOM	1262	N	ASP	A	687	17.827	62.858	-11.028	1.00	59.10	N
ATOM	1263	CA	ASP	A	687	17.628	63.859	-9.986	1.00	59.52	C
ATOM	1264	CB	ASP	A	687	18.630	65.004	-10.177	1.00	60.37	C
ATOM	1265	CG	ASP	A	687	20.073	64.562	-9.947	1.00	62.02	C
ATOM	1266	OD1	ASP	A	687	20.276	63.400	-9.533	1.00	63.03	O
ATOM	1267	OD2	ASP	A	687	21.004	65.372	-10.163	1.00	62.95	O
ATOM	1268	C	ASP	A	687	16.189	64.401	-9.936	1.00	59.77	C
ATOM	1269	O	ASP	A	687	15.621	64.581	-8.854	1.00	59.22	O
ATOM	1270	N	GLU	A	688	15.599	64.656	-11.103	1.00	60.95	N
ATOM	1271	CA	GLU	A	688	14.234	65.169	-11.163	1.00	61.11	C
ATOM	1272	CB	GLU	A	688	13.785	65.377	-12.611	1.00	63.49	C
ATOM	1273	CG	GLU	A	688	14.520	66.495	-13.343	1.00	68.06	C
ATOM	1274	CD	GLU	A	688	14.536	67.797	-12.569	1.00	70.35	C
ATOM	1275	OE1	GLU	A	688	13.564	68.034	-11.805	1.00	69.91	O
ATOM	1276	OE2	GLU	A	688	15.512	68.573	-12.741	1.00	71.37	O
ATOM	1277	C	GLU	A	688	13.281	64.215	-10.478	1.00	60.13	C
ATOM	1278	O	GLU	A	688	12.595	64.591	-9.528	1.00	60.24	O
ATOM	1279	N	ILE	A	689	13.238	62.979	-10.963	1.00	58.49	N
ATOM	1280	CA	ILE	A	689	12.358	61.964	-10.394	1.00	57.01	C
ATOM	1281	CB	ILE	A	689	12.587	60.585	-11.059	1.00	55.57	C
ATOM	1282	CG2	ILE	A	689	11.491	59.631	-10.628	1.00	55.69	C
ATOM	1283	CG1	ILE	A	689	12.574	60.727	-12.586	1.00	54.77	C
ATOM	1284	CD1	ILE	A	689	13.085	59.526	-13.347	1.00	51.65	C



ATOM	1366	CG	LYS	A	699	3.326	66.265	-0.455	1.00	47.61	C
ATOM	1367	CD	LYS	A	699	2.929	66.091	-1.910	1.00	48.03	C
ATOM	1368	CE	LYS	A	699	3.513	67.211	-2.761	1.00	49.11	C
ATOM	1369	NZ	LYS	A	699	3.239	67.074	-4.218	1.00	47.82	N
ATOM	1370	C	LYS	A	699	2.899	63.970	2.628	1.00	47.65	C
ATOM	1371	O	LYS	A	699	2.001	64.154	3.450	1.00	47.13	O
ATOM	1372	N	ALA	A	700	3.440	62.780	2.394	1.00	48.78	N
ATOM	1373	CA	ALA	A	700	2.993	61.594	3.110	1.00	50.51	C
ATOM	1374	CB	ALA	A	700	3.795	60.382	2.648	1.00	49.37	C
ATOM	1375	C	ALA	A	700	3.143	61.816	4.621	1.00	50.96	C
ATOM	1376	O	ALA	A	700	2.297	61.383	5.403	1.00	49.68	O
ATOM	1377	N	ILE	A	701	4.214	62.508	5.011	1.00	52.22	N
ATOM	1378	CA	ILE	A	701	4.478	62.812	6.413	1.00	54.71	C
ATOM	1379	CB	ILE	A	701	5.918	63.268	6.614	1.00	53.74	C
ATOM	1380	CG2	ILE	A	701	6.127	63.704	8.064	1.00	53.26	C
ATOM	1381	CG1	ILE	A	701	6.860	62.127	6.225	1.00	53.43	C
ATOM	1382	CD1	ILE	A	701	8.307	62.516	6.156	1.00	51.85	C
ATOM	1383	C	ILE	A	701	3.532	63.888	6.956	1.00	58.00	C
ATOM	1384	O	ILE	A	701	3.000	63.760	8.060	1.00	58.18	O
ATOM	1385	N	VAL	A	702	3.318	64.950	6.190	1.00	59.77	N
ATOM	1386	CA	VAL	A	702	2.409	65.993	6.637	1.00	62.49	C
ATOM	1387	CB	VAL	A	702	2.303	67.117	5.596	1.00	62.95	C
ATOM	1388	CG1	VAL	A	702	1.185	68.080	5.977	1.00	62.68	C
ATOM	1389	CG2	VAL	A	702	3.640	67.838	5.490	1.00	62.55	C
ATOM	1390	C	VAL	A	702	1.031	65.367	6.845	1.00	64.26	C
ATOM	1391	O	VAL	A	702	0.415	65.483	7.911	1.00	65.10	O
ATOM	1392	N	LYS	A	703	0.566	64.676	5.816	1.00	65.02	N
ATOM	1393	CA	LYS	A	703	-0.732	64.023	5.846	1.00	66.60	C
ATOM	1394	CB	LYS	A	703	-0.866	63.140	4.591	1.00	66.24	C
ATOM	1395	CG	LYS	A	703	-2.235	62.514	4.392	1.00	65.19	C
ATOM	1396	CD	LYS	A	703	-2.404	61.925	2.998	1.00	64.37	C
ATOM	1397	CE	LYS	A	703	-3.769	61.267	2.833	1.00	65.69	C
ATOM	1398	NZ	LYS	A	703	-3.943	60.617	1.497	1.00	65.23	N
ATOM	1399	C	LYS	A	703	-1.029	63.213	7.120	1.00	67.04	C
ATOM	1400	O	LYS	A	703	-2.179	63.063	7.496	1.00	67.09	O
ATOM	1401	N	ARG	A	704	0.008	62.715	7.790	1.00	68.03	N
ATOM	1402	CA	ARG	A	704	-0.151	61.914	9.002	1.00	68.16	C
ATOM	1403	CB	ARG	A	704	0.775	60.702	8.911	1.00	67.95	C
ATOM	1404	CG	ARG	A	704	0.950	59.888	10.175	1.00	69.89	C
ATOM	1405	CD	ARG	A	704	1.756	58.654	9.823	1.00	71.05	C
ATOM	1406	NE	ARG	A	704	2.022	57.767	10.949	1.00	73.08	N
ATOM	1407	CZ	ARG	A	704	2.870	58.029	11.942	1.00	74.45	C
ATOM	1408	NH1	ARG	A	704	3.548	59.172	11.968	1.00	75.00	N
ATOM	1409	NH2	ARG	A	704	3.061	57.126	12.900	1.00	73.60	N
ATOM	1410	C	ARG	A	704	0.108	62.697	10.282	1.00	68.04	C
ATOM	1411	O	ARG	A	704	-0.852	62.832	11.060	1.00	67.92	O
ATOM	1412	OXT	ARG	A	704	1.239	63.168	10.486	1.00	66.54	C
ATOM	1413	CB	SER	A	708	2.242	72.955	10.265	1.00	54.81	C
ATOM	1414	OG	SER	A	708	1.167	73.197	11.160	1.00	53.87	O
ATOM	1415	C	SER	A	708	2.969	71.211	11.905	1.00	57.67	C
ATOM	1416	O	SER	A	708	2.016	71.166	12.693	1.00	57.88	O
ATOM	1417	N	SER	A	708	1.758	70.564	9.773	1.00	54.28	N
ATOM	1418	CA	SER	A	708	2.732	71.508	10.411	1.00	55.76	C
ATOM	1419	N	SER	A	709	4.240	71.025	12.280	1.00	57.69	N
ATOM	1420	CA	SER	A	709	4.636	70.745	13.665	1.00	56.36	C
ATOM	1421	CB	SER	A	709	3.710	69.687	14.260	1.00	56.43	C
ATOM	1422	OG	SER	A	709	3.423	68.701	13.284	1.00	56.34	O
ATOM	1423	C	SER	A	709	6.094	70.256	13.712	1.00	57.90	C
ATOM	1424	O	SER	A	709	7.030	71.043	13.526	1.00	57.65	O
ATOM	1425	N	GLN	A	710	6.271	68.955	13.964	1.00	57.90	N
ATOM	1426	CA	GLN	A	710	7.587	68.289	14.017	1.00	56.52	C
ATOM	1427	CB	GLN	A	710	7.670	67.501	15.326	1.00	56.97	C
ATOM	1428	CG	GLN	A	710	7.116	68.329	16.512	1.00	58.60	C
ATOM	1429	CD	GLN	A	710	7.171	67.602	17.846	1.00	58.92	C
ATOM	1430	OE1	GLN	A	710	6.757	66.449	17.941	1.00	60.13	O
ATOM	1431	NE2	GLN	A	710	7.680	68.273	18.882	1.00	58.49	N
ATOM	1432	C	GLN	A	710	7.704	67.391	12.755	1.00	56.55	C
ATOM	1433	O	GLN	A	710	8.012	66.188	12.793	1.00	55.45	O
ATOM	1434	N	ASN	A	711	7.486	68.025	11.610	1.00	55.17	N
ATOM	1435	CA	ASN	A	711	7.531	67.298	10.362	1.00	56.02	C
ATOM	1436	CB	ASN	A	711	6.725	68.035	9.279	1.00	55.32	C
ATOM	1437	CG	ASN	A	711	5.251	68.271	9.658	1.00	55.98	C
ATOM	1438	OD1	ASN	A	711	4.485	68.788	8.843	1.00	55.62	O
ATOM	1439	ND2	ASN	A	711	4.856	67.895	10.878	1.00	57.73	N
ATOM	1440	C	ASN	A	711	8.932	67.009	9.838	1.00	56.20	C
ATOM	1441	O	ASN	A	711	9.129	66.038	9.106	1.00	52.71	O
ATOM	1442	N	TRP	A	712	9.915	67.823	10.201	1.00	60.06	N
ATOM	1443	CA	TRP	A	712	11.244	67.546	9.691	1.00	60.60	C
ATOM	1444	CB	TRP	A	712	12.075	68.827	9.529	1.00	62.52	C
ATOM	1445	CG	TRP	A	712	11.356	70.065	9.008	1.00	62.95	C
ATOM	1446	CD2	TRP	A	712	11.331	70.574	7.651	1.00	63.40	C

ATOM	1447	CE2	TRP	A	712	10.677	71.825	7.687	1.00	64.48	C
ATOM	1448	CE3	TRP	A	712	11.807	70.098	6.421	1.00	65.14	C
ATOM	1449	CD1	TRP	A	712	10.720	71.006	9.771	1.00	63.27	C
ATOM	1450	NE1	TRP	A	712	10.319	72.060	8.988	1.00	64.55	N
ATOM	1451	CZ2	TRP	A	712	10.485	72.612	6.551	1.00	64.85	C
ATOM	1452	CZ3	TRP	A	712	11.614	70.896	5.274	1.00	66.25	C
ATOM	1453	CH2	TRP	A	712	10.956	72.134	5.355	1.00	66.85	C
ATOM	1454	C	TRP	A	712	12.016	66.547	10.540	1.00	60.24	C
ATOM	1455	O	TRP	A	712	13.075	66.104	10.127	1.00	59.18	O
ATOM	1456	N	GLN	A	713	11.522	66.204	11.727	1.00	59.16	N
ATOM	1457	CA	GLN	A	713	12.228	65.215	12.543	1.00	57.65	C
ATOM	1458	CB	GLN	A	713	11.768	65.253	14.004	1.00	57.51	C
ATOM	1459	CG	GLN	A	713	12.558	64.312	14.916	1.00	57.90	C
ATOM	1460	CD	GLN	A	713	11.956	64.181	16.301	1.00	58.04	C
ATOM	1461	OE1	GLN	A	713	10.867	63.632	16.469	1.00	55.38	O
ATOM	1462	NE2	GLN	A	713	12.659	64.690	17.300	1.00	58.63	N
ATOM	1463	C	GLN	A	713	11.922	63.834	11.974	1.00	56.81	C
ATOM	1464	O	GLN	A	713	12.800	62.979	11.873	1.00	55.54	O
ATOM	1465	N	ARG	A	714	10.651	63.630	11.630	1.00	54.90	N
ATOM	1466	CA	ARG	A	714	10.177	62.373	11.056	1.00	54.20	C
ATOM	1467	CB	ARG	A	714	8.644	62.373	10.937	1.00	54.73	C
ATOM	1468	CG	ARG	A	714	8.080	61.063	10.409	1.00	55.69	C
ATOM	1469	CD	ARG	A	714	6.592	60.911	10.698	1.00	57.46	C
ATOM	1470	NE	ARG	A	714	6.116	59.568	10.366	1.00	55.54	N
ATOM	1471	CZ	ARG	A	714	6.494	58.464	10.999	1.00	53.99	C
ATOM	1472	NH1	ARG	A	714	7.348	58.534	12.011	1.00	50.95	N
ATOM	1473	NH2	ARG	A	714	6.037	57.287	10.601	1.00	54.37	N
ATOM	1474	C	ARG	A	714	10.801	62.214	9.674	1.00	53.10	C
ATOM	1475	O	ARG	A	714	11.170	61.112	9.262	1.00	51.84	O
ATOM	1476	N	PHE	A	715	10.921	63.329	8.961	1.00	53.44	N
ATOM	1477	CA	PHE	A	715	11.519	63.318	7.631	1.00	54.01	C
ATOM	1478	CB	PHE	A	715	11.390	64.691	6.978	1.00	53.70	C
ATOM	1479	CG	PHE	A	715	11.769	64.707	5.528	1.00	55.03	C
ATOM	1480	CD1	PHE	A	715	10.845	64.357	4.548	1.00	55.85	C
ATOM	1481	CD2	PHE	A	715	13.055	65.074	5.138	1.00	55.63	C
ATOM	1482	CE1	PHE	A	715	11.197	64.376	3.198	1.00	56.00	C
ATOM	1483	CE2	PHE	A	715	13.422	65.098	3.793	1.00	55.68	C
ATOM	1484	CZ	PHE	A	715	12.492	64.750	2.821	1.00	56.77	C
ATOM	1485	C	PHE	A	715	12.991	62.969	7.820	1.00	53.98	C
ATOM	1486	O	PHE	A	715	13.648	62.446	6.919	1.00	54.78	O
ATOM	1487	N	TYR	A	716	13.498	63.257	9.012	1.00	53.49	N
ATOM	1488	CA	TYR	A	716	14.877	62.965	9.339	1.00	52.82	C
ATOM	1489	CB	TYR	A	716	15.394	63.982	10.363	1.00	54.19	C
ATOM	1490	CG	TYR	A	716	16.811	63.747	10.828	1.00	55.32	C
ATOM	1491	CD1	TYR	A	716	17.067	63.128	12.052	1.00	55.83	C
ATOM	1492	CE1	TYR	A	716	18.368	62.896	12.485	1.00	58.40	C
ATOM	1493	CD2	TYR	A	716	17.892	64.129	10.038	1.00	55.59	C
ATOM	1494	CE2	TYR	A	716	19.198	63.903	10.451	1.00	58.23	C
ATOM	1495	CZ	TYR	A	716	19.431	63.281	11.678	1.00	60.41	C
ATOM	1496	OH	TYR	A	716	20.728	63.036	12.095	1.00	62.23	O
ATOM	1497	C	TYR	A	716	15.012	61.536	9.871	1.00	52.31	C
ATOM	1498	O	TYR	A	716	16.039	60.892	9.685	1.00	53.87	O
ATOM	1499	N	GLN	A	717	13.973	61.028	10.517	1.00	50.59	N
ATOM	1500	CA	GLN	A	717	14.011	59.678	11.040	1.00	49.14	C
ATOM	1501	CB	GLN	A	717	12.913	59.502	12.076	1.00	48.02	C
ATOM	1502	CG	GLN	A	717	13.187	60.266	13.350	1.00	47.75	C
ATOM	1503	CD	GLN	A	717	12.083	60.098	14.374	1.00	47.28	C
ATOM	1504	OE1	GLN	A	717	10.922	60.408	14.108	1.00	44.02	O
ATOM	1505	NE2	GLN	A	717	12.441	59.606	15.558	1.00	47.28	N
ATOM	1506	C	GLN	A	717	13.820	58.662	9.929	1.00	49.07	C
ATOM	1507	O	GLN	A	717	14.381	57.559	9.961	1.00	50.47	O
ATOM	1508	N	LEU	A	718	13.029	59.038	8.936	1.00	47.86	N
ATOM	1509	CA	LEU	A	718	12.749	58.133	7.840	1.00	46.90	C
ATOM	1510	CB	LEU	A	718	11.485	58.586	7.082	1.00	44.55	C
ATOM	1511	CG	LEU	A	718	10.155	58.700	7.861	1.00	42.65	C
ATOM	1512	CD1	LEU	A	718	9.009	58.733	6.873	1.00	41.64	C
ATOM	1513	CD2	LEU	A	718	9.953	57.546	8.828	1.00	37.93	C
ATOM	1514	C	LEU	A	718	13.937	58.005	6.901	1.00	46.55	C
ATOM	1515	O	LEU	A	718	14.260	56.903	6.458	1.00	45.46	O
ATOM	1516	N	THR	A	719	14.584	59.137	6.626	1.00	47.26	N
ATOM	1517	CA	THR	A	719	15.757	59.195	5.764	1.00	46.43	C
ATOM	1518	CB	THR	A	719	16.224	60.617	5.598	1.00	46.78	C
ATOM	1519	OG1	THR	A	719	15.141	61.401	5.087	1.00	49.22	O
ATOM	1520	CG2	THR	A	719	17.376	60.670	4.630	1.00	46.92	C
ATOM	1521	C	THR	A	719	16.878	58.386	6.383	1.00	46.61	C
ATOM	1522	O	THR	A	719	17.680	57.777	5.678	1.00	47.44	O
ATOM	1523	N	LYS	A	720	16.916	58.380	7.708	1.00	45.91	N
ATOM	1524	CA	LYS	A	720	17.920	57.637	8.434	1.00	46.06	C
ATOM	1525	CB	LYS	A	720	17.869	58.010	9.922	1.00	47.69	C
ATOM	1526	CG	LYS	A	720	19.064	57.537	10.738	1.00	49.40	C
ATOM	1527	CD	LYS	A	720	19.007	58.082	12.153	1.00	53.02	C

ATOM	1528	CE	LYS	A	720	20.272	57.773	12.951	1.00	53.41	C
ATOM	1529	NZ	LYS	A	720	20.138	58.236	14.374	1.00	55.37	N
ATOM	1530	C	LYS	A	720	17.692	56.132	8.244	1.00	45.84	C
ATOM	1531	O	LYS	A	720	18.623	55.401	7.917	1.00	45.91	O
ATOM	1532	N	LEU	A	721	16.461	55.666	8.439	1.00	44.81	N
ATOM	1533	CA	LEU	A	721	16.149	54.249	8.249	1.00	43.44	C
ATOM	1534	CB	LEU	A	721	14.651	54.005	8.469	1.00	44.36	C
ATOM	1535	CG	LEU	A	721	14.068	52.669	7.978	1.00	43.99	C
ATOM	1536	CD1	LEU	A	721	14.803	51.534	8.662	1.00	42.83	C
ATOM	1537	CD2	LEU	A	721	12.565	52.597	8.263	1.00	45.48	C
ATOM	1538	C	LEU	A	721	16.538	53.816	6.831	1.00	42.20	C
ATOM	1539	O	LEU	A	721	17.096	52.739	6.617	1.00	41.31	O
ATOM	1540	N	LEU	A	722	16.230	54.661	5.858	1.00	42.11	N
ATOM	1541	CA	LEU	A	722	16.563	54.351	4.482	1.00	43.13	C
ATOM	1542	CB	LEU	A	722	16.072	55.457	3.548	1.00	42.12	C
ATOM	1543	CG	LEU	A	722	14.582	55.422	3.186	1.00	42.58	C
ATOM	1544	CD1	LEU	A	722	14.212	56.630	2.337	1.00	43.09	C
ATOM	1545	CD2	LEU	A	722	14.271	54.146	2.418	1.00	43.11	C
ATOM	1546	C	LEU	A	722	18.066	54.172	4.349	1.00	44.38	C
ATOM	1547	O	LEU	A	722	18.536	53.318	3.588	1.00	44.59	O
ATOM	1548	N	ASP	A	723	18.823	54.980	5.090	1.00	45.37	N
ATOM	1549	CA	ASP	A	723	20.277	54.878	5.050	1.00	46.24	C
ATOM	1550	CB	ASP	A	723	20.947	56.097	5.693	1.00	47.55	C
ATOM	1551	CG	ASP	A	723	20.793	57.342	4.857	1.00	50.95	C
ATOM	1552	OD1	ASP	A	723	20.921	57.239	3.618	1.00	53.46	O
ATOM	1553	OD2	ASP	A	723	20.545	58.426	5.432	1.00	53.76	O
ATOM	1554	C	ASP	A	723	20.764	53.606	5.722	1.00	44.58	C
ATOM	1555	O	ASP	A	723	21.742	53.015	5.278	1.00	45.82	O
ATOM	1556	N	SER	A	724	20.088	53.175	6.783	1.00	43.57	N
ATOM	1557	CA	SER	A	724	20.496	51.952	7.465	1.00	44.04	C
ATOM	1558	CB	SER	A	724	19.844	51.848	8.843	1.00	42.14	C
ATOM	1559	OG	SER	A	724	18.583	51.201	8.784	1.00	38.58	O
ATOM	1560	C	SER	A	724	20.116	50.731	6.635	1.00	46.12	C
ATOM	1561	O	SER	A	724	20.442	49.600	6.992	1.00	47.63	O
ATOM	1562	N	MET	A	725	19.418	50.962	5.530	1.00	47.03	N
ATOM	1563	CA	MET	A	725	18.998	49.869	4.669	1.00	48.24	C
ATOM	1564	CB	MET	A	725	17.916	50.354	3.688	1.00	49.32	C
ATOM	1565	CG	MET	A	725	16.511	50.560	4.305	1.00	48.80	C
ATOM	1566	SD	MET	A	725	15.865	49.039	5.080	1.00	46.86	S
ATOM	1567	CE	MET	A	725	15.626	48.008	3.622	1.00	45.55	C
ATOM	1568	C	MET	A	725	20.193	49.328	3.898	1.00	48.98	C
ATOM	1569	O	MET	A	725	20.292	48.124	3.639	1.00	48.67	O
ATOM	1570	N	HIS	A	726	21.101	50.228	3.526	1.00	51.41	N
ATOM	1571	CA	HIS	A	726	22.299	49.854	2.766	1.00	52.22	C
ATOM	1572	CB	HIS	A	726	23.171	51.099	2.507	1.00	52.32	C
ATOM	1573	CG	HIS	A	726	24.288	50.860	1.538	1.00	55.97	C
ATOM	1574	CD2	HIS	A	726	25.639	50.851	1.709	1.00	57.37	C
ATOM	1575	ND1	HIS	A	726	24.079	50.514	0.219	1.00	55.61	N
ATOM	1576	CE1	HIS	A	726	25.231	50.297	-0.375	1.00	55.50	C
ATOM	1577	NE2	HIS	A	726	26.200	50.495	0.510	1.00	56.75	N
ATOM	1578	C	HIS	A	726	23.071	48.811	3.562	1.00	52.63	C
ATOM	1579	O	HIS	A	726	23.630	47.844	3.018	1.00	51.56	O
ATOM	1580	N	GLU	A	727	23.072	49.000	4.871	1.00	52.29	N
ATOM	1581	CA	GLU	A	727	23.773	48.078	5.730	1.00	51.66	C
ATOM	1582	CB	GLU	A	727	23.803	48.595	7.174	1.00	56.48	C
ATOM	1583	CG	GLU	A	727	24.495	49.953	7.374	1.00	61.39	C
ATOM	1584	CD	GLU	A	727	24.495	50.430	8.834	1.00	64.73	C
ATOM	1585	OE1	GLU	A	727	24.950	49.661	9.721	1.00	65.56	O
ATOM	1586	OE2	GLU	A	727	24.045	51.577	9.088	1.00	65.33	O
ATOM	1587	C	GLU	A	727	23.134	46.709	5.714	1.00	49.32	C
ATOM	1588	O	GLU	A	727	23.846	45.708	5.697	1.00	51.08	O
ATOM	1589	N	VAL	A	728	21.801	46.662	5.716	1.00	45.57	N
ATOM	1590	CA	VAL	A	728	21.061	45.397	5.743	1.00	41.94	C
ATOM	1591	CB	VAL	A	728	19.532	45.631	5.977	1.00	41.73	C
ATOM	1592	CG1	VAL	A	728	18.806	44.289	5.920	1.00	39.22	C
ATOM	1593	CG2	VAL	A	728	19.280	46.344	7.331	1.00	40.47	C
ATOM	1594	C	VAL	A	728	21.223	44.597	4.465	1.00	39.82	C
ATOM	1595	O	VAL	A	728	21.405	43.374	4.500	1.00	36.74	O
ATOM	1596	N	VAL	A	729	21.171	45.306	3.343	1.00	39.09	N
ATOM	1597	CA	VAL	A	729	21.269	44.677	2.037	1.00	41.55	C
ATOM	1598	CB	VAL	A	729	21.145	45.719	0.897	1.00	41.81	C
ATOM	1599	CG1	VAL	A	729	21.266	45.044	-0.478	1.00	40.06	C
ATOM	1600	CG2	VAL	A	729	19.819	46.415	1.013	1.00	42.70	C
ATOM	1601	C	VAL	A	729	22.536	43.893	1.857	1.00	41.95	C
ATOM	1602	O	VAL	A	729	22.520	42.865	1.205	1.00	42.16	O
ATOM	1603	N	GLU	A	730	23.632	44.388	2.414	1.00	45.51	N
ATOM	1604	CA	GLU	A	730	24.912	43.700	2.329	1.00	47.31	C
ATOM	1605	CB	GLU	A	730	25.942	44.455	3.146	1.00	53.58	C
ATOM	1606	CG	GLU	A	730	27.162	44.930	2.359	1.00	61.47	C
ATOM	1607	CD	GLU	A	730	26.983	46.313	1.744	1.00	66.80	C
ATOM	1608	OE1	GLU	A	730	27.929	46.807	1.083	1.00	69.06	O



ATOM	1690	CA	PHE	A	740	23.717	25.691	0.824	1.00	58.84	C
ATOM	1691	CB	PHE	A	740	24.275	24.753	1.916	1.00	57.34	C
ATOM	1692	CG	PHE	A	740	23.766	23.309	1.820	1.00	56.38	C
ATOM	1693	CD1	PHE	A	740	23.655	22.501	2.964	1.00	55.24	C
ATOM	1694	CD2	PHE	A	740	23.552	22.717	0.570	1.00	55.77	C
ATOM	1695	CE1	PHE	A	740	23.334	21.124	2.869	1.00	54.99	C
ATOM	1696	CE2	PHE	A	740	23.232	21.348	0.459	1.00	55.64	C
ATOM	1697	CZ	PHE	A	740	23.138	20.545	1.609	1.00	54.57	C
ATOM	1698	C	PHE	A	740	22.747	26.650	1.485	1.00	58.63	C
ATOM	1699	O	PHE	A	740	23.100	27.854	1.600	1.00	58.19	O
ATOM	1700	OXT	PHE	A	740	21.659	26.155	1.883	1.00	60.42	O
ATOM	1701	CB	THR	B	531	53.535	31.623	-7.794	1.00	52.39	C
ATOM	1702	OG1	THR	B	531	54.498	30.619	-7.453	1.00	57.33	O
ATOM	1703	CG2	THR	B	531	53.862	32.162	-9.155	1.00	53.06	C
ATOM	1704	C	THR	B	531	52.144	33.260	-6.617	1.00	52.46	C
ATOM	1705	O	THR	B	531	51.499	33.024	-5.605	1.00	53.49	O
ATOM	1706	N	THR	B	531	54.114	32.319	-5.436	1.00	50.22	N
ATOM	1707	CA	THR	B	531	53.565	32.760	-6.760	1.00	52.09	C
ATOM	1708	N	LEU	B	532	51.642	33.932	-7.642	1.00	52.61	N
ATOM	1709	CA	LEU	B	532	50.297	34.468	-7.568	1.00	51.96	C
ATOM	1710	CB	LEU	B	532	50.344	35.966	-7.867	1.00	50.92	C
ATOM	1711	CG	LEU	B	532	49.166	36.830	-7.427	1.00	50.86	C
ATOM	1712	CD1	LEU	B	532	48.523	36.249	-6.170	1.00	50.84	C
ATOM	1713	CD2	LEU	B	532	49.654	38.263	-7.217	1.00	49.30	C
ATOM	1714	C	LEU	B	532	49.371	33.716	-8.522	1.00	52.00	C
ATOM	1715	O	LEU	B	532	48.202	33.468	-8.208	1.00	54.17	O
ATOM	1716	N	VAL	B	533	49.905	33.323	-9.674	1.00	49.07	N
ATOM	1717	CA	VAL	B	533	49.118	32.572	-10.644	1.00	46.19	C
ATOM	1718	CB	VAL	B	533	49.864	32.379	-11.973	1.00	44.35	C
ATOM	1719	CG1	VAL	B	533	48.904	32.609	-13.119	1.00	39.97	C
ATOM	1720	CG2	VAL	B	533	51.059	33.297	-12.053	1.00	45.04	C
ATOM	1721	C	VAL	B	533	48.836	31.191	-10.058	1.00	46.02	C
ATOM	1722	O	VAL	B	533	47.838	30.557	-10.386	1.00	45.65	O
ATOM	1723	N	SER	B	534	49.735	30.739	-9.194	1.00	45.79	N
ATOM	1724	CA	SER	B	534	49.612	29.456	-8.519	1.00	45.42	C
ATOM	1725	CB	SER	B	534	50.850	29.257	-7.626	1.00	48.31	C
ATOM	1726	OG	SER	B	534	51.046	30.367	-6.752	1.00	49.46	O
ATOM	1727	C	SER	B	534	48.317	29.438	-7.670	1.00	44.05	C
ATOM	1728	O	SER	B	534	47.469	28.549	-7.793	1.00	42.13	O
ATOM	1729	N	LEU	B	535	48.170	30.445	-6.818	1.00	43.24	N
ATOM	1730	CA	LEU	B	535	47.000	30.557	-5.966	1.00	42.58	C
ATOM	1731	CB	LEU	B	535	47.201	31.699	-4.991	1.00	42.81	C
ATOM	1732	CG	LEU	B	535	46.191	31.831	-3.866	1.00	43.93	C
ATOM	1733	CD1	LEU	B	535	46.937	32.422	-2.683	1.00	43.21	C
ATOM	1734	CD2	LEU	B	535	44.990	32.694	-4.298	1.00	43.23	C
ATOM	1735	C	LEU	B	535	45.739	30.775	-6.808	1.00	42.64	C
ATOM	1736	O	LEU	B	535	44.624	30.486	-6.363	1.00	42.26	O
ATOM	1737	N	LEU	B	536	45.928	31.285	-8.021	1.00	40.12	N
ATOM	1738	CA	LEU	B	536	44.840	31.494	-8.952	1.00	38.89	C
ATOM	1739	CB	LEU	B	536	45.269	32.410	-10.092	1.00	37.55	C
ATOM	1740	CG	LEU	B	536	45.436	33.880	-9.739	1.00	36.50	C
ATOM	1741	CD1	LEU	B	536	45.524	34.615	-11.043	1.00	34.87	C
ATOM	1742	CD2	LEU	B	536	44.276	34.410	-8.887	1.00	33.97	C
ATOM	1743	C	LEU	B	536	44.361	30.169	-9.544	1.00	40.21	C
ATOM	1744	O	LEU	B	536	43.164	29.975	-9.760	1.00	42.19	O
ATOM	1745	N	GLU	B	537	45.290	29.262	-9.825	1.00	40.76	N
ATOM	1746	CA	GLU	B	537	44.935	27.954	-10.363	1.00	42.21	C
ATOM	1747	CB	GLU	B	537	46.191	27.193	-10.792	1.00	46.50	C
ATOM	1748	CG	GLU	B	537	46.715	27.620	-12.142	1.00	52.78	C
ATOM	1749	CD	GLU	B	537	48.122	27.132	-12.399	1.00	56.56	C
ATOM	1750	OE1	GLU	B	537	49.031	27.566	-11.655	1.00	60.08	O
ATOM	1751	OE2	GLU	B	537	48.322	26.325	-13.335	1.00	58.00	O
ATOM	1752	C	GLU	B	537	44.161	27.096	-9.360	1.00	40.58	C
ATOM	1753	O	GLU	B	537	43.294	26.317	-9.756	1.00	40.00	O
ATOM	1754	N	VAL	B	538	44.469	27.240	-8.071	1.00	38.01	N
ATOM	1755	CA	VAL	B	538	43.794	26.444	-7.054	1.00	37.67	C
ATOM	1756	CB	VAL	B	538	44.644	26.310	-5.755	1.00	37.04	C
ATOM	1757	CG1	VAL	B	538	45.952	25.588	-6.061	1.00	35.58	C
ATOM	1758	CG2	VAL	B	538	44.916	27.666	-5.162	1.00	39.11	C
ATOM	1759	C	VAL	B	538	42.414	26.971	-6.697	1.00	36.72	C
ATOM	1760	O	VAL	B	538	41.477	26.192	-6.543	1.00	38.84	O
ATOM	1761	N	ILE	B	539	42.277	28.288	-6.587	1.00	35.27	N
ATOM	1762	CA	ILE	B	539	40.991	28.880	-6.245	1.00	32.74	C
ATOM	1763	CB	ILE	B	539	41.160	30.281	-5.684	1.00	32.33	C
ATOM	1764	CG2	ILE	B	539	42.103	30.255	-4.443	1.00	28.89	C
ATOM	1765	CG1	ILE	B	539	41.568	31.211	-6.819	1.00	27.27	C
ATOM	1766	CD1	ILE	B	539	41.379	32.593	-6.429	1.00	25.41	C
ATOM	1767	C	ILE	B	539	40.031	28.971	-7.442	1.00	32.37	C
ATOM	1768	O	ILE	B	539	38.890	29.419	-7.305	1.00	31.53	O
ATOM	1769	N	GLU	B	540	40.516	28.552	-8.605	1.00	31.76	N
ATOM	1770	CA	GLU	B	540	39.733	28.548	-9.822	1.00	34.90	C

ATOM	1771	CB	GLU	B	540	40.594	28.232	-11.027	1.00	34.37	C
ATOM	1772	CG	GLU	B	540	39.810	28.224	-12.326	1.00	36.00	C
ATOM	1773	CD	GLU	B	540	39.120	29.560	-12.685	1.00	39.37	C
ATOM	1774	OE1	GLU	B	540	38.377	29.558	-13.686	1.00	42.75	O
ATOM	1775	OE2	GLU	B	540	39.297	30.612	-12.015	1.00	40.19	O
ATOM	1776	C	GLU	B	540	38.708	27.456	-9.701	1.00	36.39	C
ATOM	1777	O	GLU	B	540	39.070	26.285	-9.569	1.00	38.72	O
ATOM	1778	N	PRO	B	541	37.407	27.809	-9.754	1.00	37.28	N
ATOM	1779	CD	PRO	B	541	36.901	29.193	-9.829	1.00	35.84	C
ATOM	1780	CA	PRO	B	541	36.296	26.845	-9.646	1.00	37.87	C
ATOM	1781	CB	PRO	B	541	35.070	27.722	-9.895	1.00	37.10	C
ATOM	1782	CG	PRO	B	541	35.470	29.041	-9.345	1.00	37.64	C
ATOM	1783	C	PRO	B	541	36.402	25.671	-10.631	1.00	39.34	C
ATOM	1784	O	PRO	B	541	37.192	25.709	-11.572	1.00	39.51	O
ATOM	1785	N	GLU	B	542	35.606	24.628	-10.420	1.00	41.68	N
ATOM	1786	CA	GLU	B	542	35.626	23.453	-11.292	1.00	44.41	C
ATOM	1787	CB	GLU	B	542	35.385	22.190	-10.481	1.00	45.45	C
ATOM	1788	CG	GLU	B	542	36.320	22.065	-9.296	1.00	52.64	C
ATOM	1789	CD	GLU	B	542	36.239	20.709	-8.601	1.00	55.59	C
ATOM	1790	OE1	GLU	B	542	35.168	20.380	-8.045	1.00	57.23	O
ATOM	1791	OE2	GLU	B	542	37.248	19.965	-8.602	1.00	56.53	O
ATOM	1792	C	GLU	B	542	34.524	23.594	-12.305	1.00	44.81	C
ATOM	1793	O	GLU	B	542	33.497	24.177	-12.004	1.00	46.84	O
ATOM	1794	N	VAL	B	543	34.716	23.051	-13.497	1.00	44.00	N
ATOM	1795	CA	VAL	B	543	33.697	23.154	-14.517	1.00	45.77	C
ATOM	1796	CB	VAL	B	543	34.148	22.486	-15.802	1.00	46.89	C
ATOM	1797	CG1	VAL	B	543	35.156	23.406	-16.532	1.00	48.10	C
ATOM	1798	CG2	VAL	B	543	34.769	21.112	-15.467	1.00	51.04	C
ATOM	1799	C	VAL	B	543	32.372	22.542	-14.087	1.00	46.09	C
ATOM	1800	O	VAL	B	543	32.187	21.329	-14.148	1.00	46.57	O
ATOM	1801	N	LEU	B	544	31.436	23.385	-13.658	1.00	46.41	N
ATOM	1802	CA	LEU	B	544	30.136	22.885	-13.244	1.00	47.24	C
ATOM	1803	CB	LEU	B	544	29.283	24.003	-12.664	1.00	43.60	C
ATOM	1804	CG	LEU	B	544	29.687	24.562	-11.302	1.00	43.48	C
ATOM	1805	CD1	LEU	B	544	28.872	25.854	-10.958	1.00	42.42	C
ATOM	1806	CD2	LEU	B	544	29.506	23.453	-10.270	1.00	41.55	C
ATOM	1807	C	LEU	B	544	29.379	22.204	-14.388	1.00	49.87	C
ATOM	1808	O	LEU	B	544	29.517	22.561	-15.558	1.00	50.23	O
ATOM	1809	N	TYR	B	545	28.560	21.219	-14.037	1.00	52.75	N
ATOM	1810	CA	TYR	B	545	27.773	20.509	-15.034	1.00	52.89	C
ATOM	1811	CB	TYR	B	545	27.756	19.020	-14.730	1.00	53.87	C
ATOM	1812	CG	TYR	B	545	28.930	18.285	-15.315	1.00	53.89	C
ATOM	1813	CD1	TYR	B	545	28.835	17.692	-16.568	1.00	53.83	C
ATOM	1814	CE1	TYR	B	545	29.916	17.040	-17.138	1.00	54.82	C
ATOM	1815	CD2	TYR	B	545	30.148	18.211	-14.637	1.00	53.16	C
ATOM	1816	CE2	TYR	B	545	31.248	17.557	-15.206	1.00	53.59	C
ATOM	1817	CZ	TYR	B	545	31.119	16.976	-16.458	1.00	54.13	C
ATOM	1818	OH	TYR	B	545	32.178	16.322	-17.041	1.00	54.34	O
ATOM	1819	C	TYR	B	545	26.369	21.038	-15.023	1.00	53.05	C
ATOM	1820	O	TYR	B	545	25.901	21.526	-13.998	1.00	52.36	O
ATOM	1821	N	ALA	B	546	25.705	20.934	-16.168	1.00	55.27	N
ATOM	1822	CA	ALA	B	546	24.322	21.381	-16.328	1.00	58.49	C
ATOM	1823	CB	ALA	B	546	24.136	22.003	-17.719	1.00	59.10	C
ATOM	1824	C	ALA	B	546	23.317	20.238	-16.143	1.00	59.76	C
ATOM	1825	O	ALA	B	546	22.175	20.466	-15.743	1.00	60.66	O
ATOM	1826	N	GLY	B	547	23.748	19.014	-16.438	1.00	60.65	N
ATOM	1827	CA	GLY	B	547	22.856	17.873	-16.322	1.00	60.96	C
ATOM	1828	C	GLY	B	547	21.720	17.986	-17.326	1.00	60.72	C
ATOM	1829	O	GLY	B	547	20.659	17.399	-17.147	1.00	59.16	O
ATOM	1830	N	TYR	B	548	21.940	18.753	-18.387	1.00	61.52	N
ATOM	1831	CA	TYR	B	548	20.921	18.923	-19.396	1.00	62.74	C
ATOM	1832	CB	TYR	B	548	21.398	19.855	-20.484	1.00	59.18	C
ATOM	1833	CG	TYR	B	548	20.380	20.087	-21.563	1.00	55.17	C
ATOM	1834	CD1	TYR	B	548	20.375	19.305	-22.720	1.00	53.99	C
ATOM	1835	CE1	TYR	B	548	19.487	19.559	-23.751	1.00	51.38	C
ATOM	1836	CD2	TYR	B	548	19.457	21.123	-21.458	1.00	51.90	C
ATOM	1837	CE2	TYR	B	548	18.557	21.384	-22.492	1.00	49.83	C
ATOM	1838	CZ	TYR	B	548	18.583	20.592	-23.638	1.00	48.86	C
ATOM	1839	OH	TYR	B	548	17.736	20.804	-24.694	1.00	46.76	O
ATOM	1840	C	TYR	B	548	20.562	17.590	-20.011	1.00	66.31	C
ATOM	1841	O	TYR	B	548	21.442	16.799	-20.358	1.00	66.88	O
ATOM	1842	N	ASP	B	549	19.257	17.365	-20.145	1.00	69.27	N
ATOM	1843	CA	ASP	B	549	18.704	16.152	-20.716	1.00	71.55	C
ATOM	1844	CB	ASP	B	549	17.170	16.149	-20.561	1.00	73.15	C
ATOM	1845	CG	ASP	B	549	16.514	17.480	-20.973	1.00	74.14	C
ATOM	1846	OD1	ASP	B	549	16.259	17.711	-22.182	1.00	73.77	O
ATOM	1847	OD2	ASP	B	549	16.250	18.301	-20.063	1.00	74.24	O
ATOM	1848	C	ASP	B	549	19.063	15.983	-22.176	1.00	73.19	C
ATOM	1849	O	ASP	B	549	18.379	16.515	-23.055	1.00	73.92	O
ATOM	1850	N	SER	B	550	20.148	15.260	-22.438	1.00	74.98	N
ATOM	1851	CA	SER	B	550	20.549	14.990	-23.815	1.00	76.61	C









































ATOM	3472	O30	486	E	1	13.467	33.663	-13.116	1.00	37.11
ATOM	3473	C30	486	E	1	18.364	42.330	-11.163	1.00	31.67
ATOM	3474	C31	486	E	1	19.414	41.686	-11.129	1.00	33.64
ATOM	3475	C32	486	E	1	17.218	43.271	-11.355	1.00	24.92
ATOM	3476	O	WAT	X	1	9.283	41.417	-0.469	1.00	29.28
ATOM	3477	O	WAT	X	2	28.937	25.308	-16.720	1.00	36.08
END										

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REMARK 3 REFINEMENT.
REMARK 3 PROGRAM : CNX 2000.1
REMARK 3 AUTHORS : Brunger, Adams, Clore, Delano,
REMARK 3 Gros, Grosse-Kunstleve, Jiang,
REMARK 3 Kuszewski, Nilges, Pannu, Read,
REMARK 3 Rice, Simonson, Warren
REMARK 3 and
REMARK 3 Molecular Simulations Inc.,
REMARK 3 (Badger, Berard, Kumar, Szalma,
REMARK 3 Yip).
REMARK 3
REMARK 3 DATA USED IN REFINEMENT.
REMARK 3 RESOLUTION RANGE HIGH (ANGSTROMS) : 2.80
REMARK 3 RESOLUTION RANGE LOW (ANGSTROMS) : 37.27
REMARK 3 DATA CUTOFF (SIGMA(F)) : 0.0
REMARK 3 DATA CUTOFF HIGH (ABS(F)) : 973340.75
REMARK 3 DATA CUTOFF LOW (ABS(F)) : 0.000000
REMARK 3 COMPLETENESS (WORKING+TEST) (%) : 98.2
REMARK 3 NUMBER OF REFLECTIONS : 8219
REMARK 3
REMARK 3 FIT TO DATA USED IN REFINEMENT.
REMARK 3 CROSS-VALIDATION METHOD : THROUGHOUT
REMARK 3 FREE R VALUE TEST SET SELECTION : RANDOM
REMARK 3 R VALUE (WORKING SET) : 0.220
REMARK 3 FREE R VALUE : 0.262
REMARK 3 FREE R VALUE TEST SET SIZE (%) : 5.0
REMARK 3 FREE R VALUE TEST SET COUNT : 414
REMARK 3 ESTIMATED ERROR OF FREE R VALUE : 0.013
REMARK 3
REMARK 3 FIT IN THE HIGHEST RESOLUTION BIN.
REMARK 3 TOTAL NUMBER OF BINS USED : 6
REMARK 3 BIN RESOLUTION RANGE HIGH (A) : 2.80
REMARK 3 BIN RESOLUTION RANGE LOW (A) : 2.98
REMARK 3 BIN COMPLETENESS (WORKING+TEST) (%) : 97.2
REMARK 3 REFLECTIONS IN BIN (WORKING SET) : 1245
REMARK 3 BIN R VALUE (WORKING SET) : 0.287
REMARK 3 BIN FREE R VALUE : 0.323
REMARK 3 BIN FREE R VALUE TEST SET SIZE (%) : 5.0
REMARK 3 BIN FREE R VALUE TEST SET COUNT : 65
REMARK 3 ESTIMATED ERROR OF BIN FREE R VALUE : 0.040
REMARK 3
REMARK 3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK 3 PROTEIN ATOMS : 2026
REMARK 3 NUCLEIC ACID ATOMS : 0
REMARK 3 HETEROGEN ATOMS : 0
REMARK 3 SOLVENT ATOMS : 0
REMARK 3
REMARK 3 B VALUES.
REMARK 3 FROM WILSON PLOT (A**2) : 19.6
REMARK 3 MEAN B VALUE (OVERALL, A**2) : 33.6
REMARK 3 OVERALL ANISOTROPIC B VALUE.
REMARK 3 B11 (A**2) : 1.60
REMARK 3 B22 (A**2) : 12.50
REMARK 3 B33 (A**2) : -14.10
REMARK 3 B12 (A**2) : 0.00
REMARK 3 B13 (A**2) : 0.00
REMARK 3 B23 (A**2) : 0.00
REMARK 3
REMARK 3 BULK SOLVENT MODELING.
REMARK 3 METHOD USED : FLAT MODEL
REMARK 3 KSOL : 0.350747
REMARK 3 BSOL : 21.401 (A**2)
REMARK 3

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REMARK 3 ESTIMATED COORDINATE ERROR.
REMARK 3 ESD FROM LUZZATI PLOT (A) : 0.34
REMARK 3 ESD FROM SIGMAA (A) : 0.33
REMARK 3 LOW RESOLUTION CUTOFF (A) : 5.00
REMARK 3
REMARK 3 CROSS-VALIDATED ESTIMATED COORDINATE ERROR.
REMARK 3 ESD FROM C-V LUZZATI PLOT (A) : 0.45
REMARK 3 ESD FROM C-V SIGMAA (A) : 0.29
REMARK 3
REMARK 3 RMS DEVIATIONS FROM IDEAL VALUES.
REMARK 3 BOND LENGTHS (A) : 0.008
REMARK 3 BOND ANGLES (DEGREES) : 1.1
REMARK 3 DIHEDRAL ANGLES (DEGREES) : 18.9
REMARK 3 IMPROPER ANGLES (DEGREES) : 0.73
REMARK 3
REMARK 3 ISOTROPIC THERMAL MODEL : RESTRAINED
REMARK 3
REMARK 3 ISOTROPIC THERMAL FACTOR RESTRAINTS. RMS SIGMA
REMARK 3 MAIN-CHAIN BOND (A**2) : 1.46 ; 1.50
REMARK 3 MAIN-CHAIN ANGLE (A**2) : 2.54 ; 2.00
REMARK 3 SIDE-CHAIN BOND (A**2) : 2.06 ; 2.00
REMARK 3 SIDE-CHAIN ANGLE (A**2) : 3.09 ; 2.50
REMARK 3
REMARK 3 NCS MODEL : NONE
REMARK 3
REMARK 3 NCS RESTRAINTS. RMS
SIGMA/WEIGHT
REMARK 3 GROUP 1 POSITIONAL (A) : NULL ; NULL
REMARK 3 GROUP 1 B-FACTOR (A**2) : NULL ; NULL
REMARK 3
REMARK 3 PARAMETER FILE 1 : MSI_CNX_TOPPAR/protein_rep.param
REMARK 3 PARAMETER FILE 2 : MSI_CNX_TOPPAR/water_rep.param
REMARK 3 PARAMETER FILE 3 : ligands.par
REMARK 3 TOPOLOGY FILE 1 : MSI_CNX_TOPPAR/protein.top
REMARK 3 TOPOLOGY FILE 2 : MSI_CNX_TOPPAR/water.top
REMARK 3 TOPOLOGY FILE 3 : ligands.top
REMARK 3
REMARK 3 OTHER REFINEMENT REMARKS: NULL
SEQRES 1 A 261 PRO THR LEU VAL SER LEU LEU GLU VAL ILE GLU PRO GLU
SEQRES 2 A 261 VAL LEU TYR ALA GLY TYR ASP SER SER VAL PRO ASP SER
SEQRES 3 A 261 THR TRP ARG ILE MET THR THR LEU ASN MET LEU GLY GLY
SEQRES 4 A 261 ARG GLN VAL ILE ALA ALA VAL LYS TRP ALA LYS ALA ILE
SEQRES 5 A 261 PRO GLY PHE ARG ASN LEU HIS LEU ASP ASP GLN MET THR
SEQRES 6 A 261 LEU LEU GLN TYR SER TRP MET SER LEU MET ALA PHE ALA
SEQRES 7 A 261 LEU GLY TRP ARG SER TYR ARG GLN SER SER ALA ASN LEU
SEQRES 8 A 261 LEU CYS PHE ALA PRO ASP LEU ILE ILE ASN GLU GLN ARG
SEQRES 9 A 261 MET THR LEU PRO ASP MET TYR ASP GLN CYS LYS HIS MET
SEQRES 10 A 261 LEU TYR VAL SER SER GLU LEU HIS ARG LEU GLN VAL SER
SEQRES 11 A 261 TYR GLU GLU TYR LEU CYS MET LYS THR LEU LEU LEU LEU
SEQRES 12 A 261 SER SER VAL PRO LYS ASP GLY LEU LYS SER GLN GLU LEU
SEQRES 13 A 261 PHE ASP GLU ILE ARG MET THR TYR ILE LYS GLU LEU GLY
SEQRES 14 A 261 LYS ALA ILE VAL LYS ARG GLU GLY ASN SER SER GLN ASN
SEQRES 15 A 261 TRP GLN ARG PHE TYR GLN LEU THR LYS LEU LEU ASP SER
SEQRES 16 A 261 MET HIS GLU VAL VAL GLU ASN LEU LEU ASN TYR CYS PHE
SEQRES 17 A 261 GLN THR PHE LEU ASP LYS THR MET SER ILE GLU PHE PRO
SEQRES 18 A 261 GLU MET LEU ALA GLU ILE ILE THR ASN ASN ILE LYS LYS
SEQRES 19 A 261 LEU LEU PHE HIS GLN 486 HXD HXD HXD HOH HOH HOH HOH
SEQRES 20 A 261 HOH HOH HOH HOH HOH HOH HOH HOH HOH HOH HOH HOH
SEQRES 21 A 261 HOH
CRYST1 74.541 109.686 39.120 90.00 90.00 90.00 P 21 21 2
4
ORIGX1 1.000000 0.000000 0.000000 0.000000
ORIGX2 0.000000 1.000000 0.000000 0.000000
ORIGX3 0.000000 0.000000 1.000000 0.000000
SCALE1 0.013415 0.000000 0.000000 0.000000
SCALE2 0.000000 0.009117 0.000000 0.000000

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SCALE3	0.000000	0.000000	0.025562	0.000000					
ATOM	1	CB	PRO A 530	0.065	41.107	-12.883	1.00	55.78	C
ATOM	2	CG	PRO A 530	-0.726	41.877	-13.946	1.00	56.26	C
ATOM	3	C	PRO A 530	2.373	41.506	-11.971	1.00	53.10	C
ATOM	4	O	PRO A 530	3.130	40.944	-12.772	1.00	52.07	O
ATOM	5	N	PRO A 530	1.275	43.083	-13.591	1.00	55.71	N
ATOM	6	CD	PRO A 530	0.339	42.734	-14.678	1.00	56.36	C
ATOM	7	CA	PRO A 530	1.074	42.164	-12.440	1.00	54.71	C
ATOM	8	N	THR A 531	2.622	41.589	-10.667	1.00	51.23	N
ATOM	9	CA	THR A 531	3.810	41.001	-10.062	1.00	48.81	C
ATOM	10	CB	THR A 531	3.951	41.420	-8.589	1.00	48.90	C
ATOM	11	OG1	THR A 531	2.852	40.892	-7.836	1.00	48.07	O
ATOM	12	CG2	THR A 531	3.952	42.930	-8.470	1.00	47.66	C
ATOM	13	C	THR A 531	3.696	39.483	-10.116	1.00	47.13	C
ATOM	14	O	THR A 531	2.633	38.940	-10.425	1.00	46.33	O
ATOM	15	N	LEU A 532	4.788	38.799	-9.804	1.00	45.00	N
ATOM	16	CA	LEU A 532	4.786	37.345	-9.831	1.00	42.64	C
ATOM	17	CB	LEU A 532	6.221	36.820	-9.834	1.00	42.31	C
ATOM	18	CG	LEU A 532	6.381	35.352	-10.228	1.00	43.18	C
ATOM	19	CD1	LEU A 532	5.607	35.075	-11.511	1.00	43.25	C
ATOM	20	CD2	LEU A 532	7.863	35.036	-10.400	1.00	42.81	C
ATOM	21	C	LEU A 532	4.012	36.752	-8.658	1.00	41.18	C
ATOM	22	O	LEU A 532	3.355	35.725	-8.806	1.00	40.72	O
ATOM	23	N	VAL A 533	4.081	37.396	-7.496	1.00	39.79	N
ATOM	24	CA	VAL A 533	3.365	36.893	-6.326	1.00	40.05	C
ATOM	25	CB	VAL A 533	3.807	37.598	-5.039	1.00	39.97	C
ATOM	26	CG1	VAL A 533	5.085	36.975	-4.531	1.00	40.52	C
ATOM	27	CG2	VAL A 533	3.995	39.076	-5.300	1.00	39.84	C
ATOM	28	C	VAL A 533	1.859	37.048	-6.464	1.00	39.08	C
ATOM	29	O	VAL A 533	1.097	36.222	-5.970	1.00	37.55	O
ATOM	30	N	SER A 534	1.432	38.111	-7.132	1.00	38.96	N
ATOM	31	CA	SER A 534	0.010	38.335	-7.336	1.00	39.75	C
ATOM	32	CB	SER A 534	-0.233	39.690	-8.027	1.00	40.51	C
ATOM	33	OG	SER A 534	0.385	39.759	-9.301	1.00	41.31	O
ATOM	34	C	SER A 534	-0.539	37.188	-8.185	1.00	39.54	C
ATOM	35	O	SER A 534	-1.627	36.678	-7.933	1.00	40.08	O
ATOM	36	N	LEU A 535	0.231	36.770	-9.183	1.00	39.56	N
ATOM	37	CA	LEU A 535	-0.190	35.680	-10.044	1.00	39.53	C
ATOM	38	CB	LEU A 535	0.806	35.493	-11.190	1.00	41.20	C
ATOM	39	CG	LEU A 535	1.095	36.768	-11.991	1.00	43.98	C
ATOM	40	CD1	LEU A 535	2.035	36.437	-13.138	1.00	43.94	C
ATOM	41	CD2	LEU A 535	-0.202	37.376	-12.518	1.00	43.10	C
ATOM	42	C	LEU A 535	-0.292	34.402	-9.221	1.00	39.02	C
ATOM	43	O	LEU A 535	-1.264	33.659	-9.338	1.00	39.90	O
ATOM	44	N	LEU A 536	0.714	34.147	-8.390	1.00	37.12	N
ATOM	45	CA	LEU A 536	0.709	32.959	-7.541	1.00	35.80	C
ATOM	46	CB	LEU A 536	1.955	32.921	-6.649	1.00	34.24	C
ATOM	47	CG	LEU A 536	3.311	32.679	-7.303	1.00	33.46	C
ATOM	48	CD1	LEU A 536	4.409	32.680	-6.248	1.00	31.34	C
ATOM	49	CD2	LEU A 536	3.277	31.348	-8.020	1.00	34.15	C
ATOM	50	C	LEU A 536	-0.537	32.922	-6.655	1.00	35.21	C
ATOM	51	O	LEU A 536	-1.063	31.849	-6.358	1.00	33.62	O
ATOM	52	N	GLU A 537	-1.004	34.094	-6.231	1.00	34.84	N
ATOM	53	CA	GLU A 537	-2.182	34.155	-5.379	1.00	35.83	C
ATOM	54	CB	GLU A 537	-2.396	35.562	-4.831	1.00	36.63	C
ATOM	55	CG	GLU A 537	-3.583	35.631	-3.872	1.00	41.37	C
ATOM	56	CD	GLU A 537	-3.783	37.007	-3.263	1.00	43.48	C
ATOM	57	OE1	GLU A 537	-2.768	37.693	-3.006	1.00	45.77	O
ATOM	58	OE2	GLU A 537	-4.950	37.392	-3.025	1.00	43.83	O
ATOM	59	C	GLU A 537	-3.446	33.722	-6.106	1.00	35.89	C
ATOM	60	O	GLU A 537	-4.244	32.945	-5.576	1.00	36.35	O
ATOM	61	N	VAL A 538	-3.633	34.221	-7.322	1.00	34.25	N
ATOM	62	CA	VAL A 538	-4.820	33.869	-8.061	1.00	34.53	C

ATOM	63	CB	VAL	A	538	-4.948	34.699	-9.375	1.00	36.03	C
ATOM	64	CG1	VAL	A	538	-4.662	36.168	-9.083	1.00	36.24	C
ATOM	65	CG2	VAL	A	538	-4.030	34.161	-10.449	1.00	36.46	C
ATOM	66	C	VAL	A	538	-4.887	32.376	-8.376	1.00	33.99	C
ATOM	67	O	VAL	A	538	-5.965	31.790	-8.333	1.00	35.66	O
ATOM	68	N	ILE	A	539	-3.752	31.749	-8.675	1.00	32.13	N
ATOM	69	CA	ILE	A	539	-3.776	30.325	-8.998	1.00	31.87	C
ATOM	70	CB	ILE	A	539	-2.562	29.891	-9.861	1.00	32.38	C
ATOM	71	CG2	ILE	A	539	-2.523	30.718	-11.146	1.00	31.58	C
ATOM	72	CG1	ILE	A	539	-1.264	30.003	-9.046	1.00	29.84	C
ATOM	73	CD1	ILE	A	539	-0.029	29.484	-9.774	1.00	26.75	C
ATOM	74	C	ILE	A	539	-3.812	29.439	-7.761	1.00	31.94	C
ATOM	75	O	ILE	A	539	-4.004	28.230	-7.870	1.00	32.56	O
ATOM	76	N	GLU	A	540	-3.631	30.036	-6.588	1.00	31.90	N
ATOM	77	CA	GLU	A	540	-3.654	29.274	-5.345	1.00	32.09	C
ATOM	78	CB	GLU	A	540	-3.430	30.213	-4.154	1.00	31.62	C
ATOM	79	CG	GLU	A	540	-3.398	29.515	-2.802	1.00	31.44	C
ATOM	80	CD	GLU	A	540	-2.309	28.454	-2.687	1.00	32.18	C
ATOM	81	OE1	GLU	A	540	-2.357	27.677	-1.705	1.00	34.64	O
ATOM	82	OE2	GLU	A	540	-1.410	28.396	-3.557	1.00	28.36	O
ATOM	83	C	GLU	A	540	-4.996	28.534	-5.220	1.00	32.25	C
ATOM	84	O	GLU	A	540	-6.064	29.143	-5.307	1.00	31.84	O
ATOM	85	N	PRO	A	541	-4.951	27.203	-5.024	1.00	32.48	N
ATOM	86	CD	PRO	A	541	-3.738	26.368	-4.958	1.00	32.78	C
ATOM	87	CA	PRO	A	541	-6.150	26.367	-4.896	1.00	31.46	C
ATOM	88	CB	PRO	A	541	-5.575	24.962	-4.690	1.00	30.60	C
ATOM	89	CG	PRO	A	541	-4.268	25.015	-5.385	1.00	31.94	C
ATOM	90	C	PRO	A	541	-7.109	26.745	-3.772	1.00	31.92	C
ATOM	91	O	PRO	A	541	-6.715	27.265	-2.735	1.00	31.71	O
ATOM	92	N	GLU	A	542	-8.388	26.484	-4.001	1.00	34.35	N
ATOM	93	CA	GLU	A	542	-9.407	26.735	-2.995	1.00	33.34	C
ATOM	94	CB	GLU	A	542	-10.801	26.754	-3.636	1.00	35.18	C
ATOM	95	CG	GLU	A	542	-11.230	28.120	-4.144	1.00	40.83	C
ATOM	96	CD	GLU	A	542	-12.267	28.032	-5.248	1.00	44.57	C
ATOM	97	OE1	GLU	A	542	-13.316	27.386	-5.033	1.00	47.56	O
ATOM	98	OE2	GLU	A	542	-12.032	28.607	-6.333	1.00	47.08	O
ATOM	99	C	GLU	A	542	-9.283	25.557	-2.042	1.00	31.02	C
ATOM	100	O	GLU	A	542	-8.798	24.489	-2.433	1.00	28.04	O
ATOM	101	N	VAL	A	543	-9.704	25.756	-0.798	1.00	29.63	N
ATOM	102	CA	VAL	A	543	-9.633	24.703	0.199	1.00	30.09	C
ATOM	103	CB	VAL	A	543	-9.753	25.279	1.624	1.00	29.86	C
ATOM	104	CG1	VAL	A	543	-11.072	26.060	1.764	1.00	34.84	C
ATOM	105	CG2	VAL	A	543	-9.680	24.155	2.639	1.00	28.98	C
ATOM	106	C	VAL	A	543	-10.760	23.718	-0.054	1.00	29.81	C
ATOM	107	O	VAL	A	543	-11.922	24.110	-0.144	1.00	33.37	O
ATOM	108	N	LEU	A	544	-10.412	22.443	-0.185	1.00	28.80	N
ATOM	109	CA	LEU	A	544	-11.395	21.394	-0.444	1.00	28.29	C
ATOM	110	CB	LEU	A	544	-10.739	20.231	-1.208	1.00	26.52	C
ATOM	111	CG	LEU	A	544	-10.064	20.520	-2.552	1.00	25.75	C
ATOM	112	CD1	LEU	A	544	-9.540	19.212	-3.182	1.00	26.63	C
ATOM	113	CD2	LEU	A	544	-11.064	21.175	-3.477	1.00	24.27	C
ATOM	114	C	LEU	A	544	-11.983	20.856	0.854	1.00	27.42	C
ATOM	115	O	LEU	A	544	-11.359	20.961	1.908	1.00	28.33	O
ATOM	116	N	TYR	A	545	-13.183	20.283	0.771	1.00	27.60	N
ATOM	117	CA	TYR	A	545	-13.846	19.689	1.931	1.00	27.84	C
ATOM	118	CB	TYR	A	545	-15.355	19.868	1.836	1.00	28.96	C
ATOM	119	CG	TYR	A	545	-15.838	21.220	2.292	1.00	30.17	C
ATOM	120	CD1	TYR	A	545	-16.343	21.399	3.581	1.00	29.47	C
ATOM	121	CE1	TYR	A	545	-16.736	22.658	4.034	1.00	29.92	C
ATOM	122	CD2	TYR	A	545	-15.740	22.335	1.458	1.00	28.88	C
ATOM	123	CE2	TYR	A	545	-16.131	23.603	1.902	1.00	28.62	C
ATOM	124	CZ	TYR	A	545	-16.624	23.756	3.192	1.00	29.32	C
ATOM	125	OH	TYR	A	545	-16.988	25.000	3.655	1.00	28.97	O
ATOM	126	C	TYR	A	545	-13.526	18.204	1.944	1.00	28.67	C
ATOM	127	O	TYR	A	545	-13.223	17.631	0.901	1.00	31.08	O
ATOM	128	N	ALA	A	546	-13.600	17.577	3.113	1.00	28.25	N

ATOM	129	CA	ALA	A	546	-13.313	16.153	3.225	1.00	30.01	C
ATOM	130	CB	ALA	A	546	-12.777	15.836	4.607	1.00	28.48	C
ATOM	131	C	ALA	A	546	-14.540	15.294	2.944	1.00	33.68	C
ATOM	132	O	ALA	A	546	-14.439	14.244	2.299	1.00	34.22	O
ATOM	133	N	GLY	A	547	-15.695	15.747	3.427	1.00	35.63	N
ATOM	134	CA	GLY	A	547	-16.922	14.999	3.238	1.00	38.13	C
ATOM	135	C	GLY	A	547	-17.131	14.122	4.454	1.00	42.00	C
ATOM	136	O	GLY	A	547	-17.980	13.231	4.463	1.00	43.45	O
ATOM	137	N	TYR	A	548	-16.340	14.389	5.490	1.00	44.22	N
ATOM	138	CA	TYR	A	548	-16.392	13.645	6.744	1.00	45.12	C
ATOM	139	CB	TYR	A	548	-15.060	13.808	7.492	1.00	41.21	C
ATOM	140	CG	TYR	A	548	-14.909	12.932	8.717	1.00	38.15	C
ATOM	141	CD1	TYR	A	548	-15.465	13.304	9.943	1.00	37.55	C
ATOM	142	CE1	TYR	A	548	-15.311	12.503	11.078	1.00	36.26	C
ATOM	143	CD2	TYR	A	548	-14.200	11.733	8.655	1.00	35.84	C
ATOM	144	CE2	TYR	A	548	-14.042	10.924	9.778	1.00	36.04	C
ATOM	145	CZ	TYR	A	548	-14.597	11.315	10.992	1.00	36.31	C
ATOM	146	OH	TYR	A	548	-14.413	10.538	12.121	1.00	34.00	O
ATOM	147	C	TYR	A	548	-17.537	14.156	7.608	1.00	48.53	C
ATOM	148	O	TYR	A	548	-17.638	15.362	7.871	1.00	49.58	O
ATOM	149	N	ASP	A	549	-18.409	13.248	8.040	1.00	51.49	N
ATOM	150	CA	ASP	A	549	-19.520	13.653	8.888	1.00	54.98	C
ATOM	151	CB	ASP	A	549	-20.853	13.108	8.361	1.00	57.65	C
ATOM	152	CG	ASP	A	549	-22.055	13.875	8.917	1.00	59.27	C
ATOM	153	OD1	ASP	A	549	-22.281	13.837	10.145	1.00	57.39	O
ATOM	154	OD2	ASP	A	549	-22.770	14.526	8.122	1.00	62.37	O
ATOM	155	C	ASP	A	549	-19.315	13.217	10.335	1.00	55.61	C
ATOM	156	O	ASP	A	549	-19.085	12.039	10.634	1.00	53.35	O
ATOM	157	N	SER	A	550	-19.395	14.206	11.219	1.00	57.27	N
ATOM	158	CA	SER	A	550	-19.227	14.024	12.650	1.00	58.87	C
ATOM	159	CB	SER	A	550	-19.162	15.397	13.314	1.00	58.42	C
ATOM	160	OG	SER	A	550	-20.270	16.189	12.923	1.00	56.75	O
ATOM	161	C	SER	A	550	-20.348	13.194	13.289	1.00	61.02	C
ATOM	162	O	SER	A	550	-20.299	12.892	14.485	1.00	61.52	O
ATOM	163	N	SER	A	551	-21.353	12.831	12.495	1.00	62.10	N
ATOM	164	CA	SER	A	551	-22.476	12.044	12.996	1.00	63.26	C
ATOM	165	CB	SER	A	551	-23.420	11.668	11.847	1.00	63.85	C
ATOM	166	OG	SER	A	551	-22.747	10.933	10.836	1.00	65.85	O
ATOM	167	C	SER	A	551	-21.960	10.786	13.683	1.00	63.82	C
ATOM	168	O	SER	A	551	-21.984	10.680	14.915	1.00	63.91	O
ATOM	169	N	VAL	A	552	-21.494	9.834	12.881	1.00	63.85	N
ATOM	170	CA	VAL	A	552	-20.952	8.592	13.416	1.00	63.41	C
ATOM	171	CB	VAL	A	552	-20.630	7.585	12.290	1.00	64.14	C
ATOM	172	CG1	VAL	A	552	-20.101	6.289	12.884	1.00	64.09	C
ATOM	173	CG2	VAL	A	552	-21.879	7.320	11.458	1.00	65.52	C
ATOM	174	C	VAL	A	552	-19.665	8.926	14.168	1.00	61.57	C
ATOM	175	O	VAL	A	552	-18.848	9.728	13.703	1.00	61.73	O
ATOM	176	N	PRO	A	553	-19.476	8.321	15.349	1.00	59.49	N
ATOM	177	CD	PRO	A	553	-20.368	7.354	16.014	1.00	59.31	C
ATOM	178	CA	PRO	A	553	-18.279	8.567	16.157	1.00	57.83	C
ATOM	179	CB	PRO	A	553	-18.399	7.522	17.267	1.00	59.00	C
ATOM	180	CG	PRO	A	553	-19.886	7.410	17.446	1.00	59.06	C
ATOM	181	C	PRO	A	553	-16.993	8.416	15.345	1.00	55.03	C
ATOM	182	O	PRO	A	553	-16.949	7.673	14.361	1.00	54.34	O
ATOM	183	N	ASP	A	554	-15.948	9.125	15.755	1.00	52.28	N
ATOM	184	CA	ASP	A	554	-14.679	9.042	15.046	1.00	50.09	C
ATOM	185	CB	ASP	A	554	-13.626	9.941	15.690	1.00	50.05	C
ATOM	186	CG	ASP	A	554	-13.965	11.397	15.566	1.00	51.10	C
ATOM	187	OD1	ASP	A	554	-14.499	11.777	14.504	1.00	53.34	O
ATOM	188	OD2	ASP	A	554	-13.694	12.161	16.519	1.00	52.08	O
ATOM	189	C	ASP	A	554	-14.153	7.621	15.003	1.00	47.37	C
ATOM	190	O	ASP	A	554	-14.538	6.774	15.801	1.00	46.96	O
ATOM	191	N	SER	A	555	-13.258	7.379	14.061	1.00	45.53	N
ATOM	192	CA	SER	A	555	-12.653	6.073	13.878	1.00	43.89	C
ATOM	193	CB	SER	A	555	-13.616	5.163	13.115	1.00	42.57	C
ATOM	194	OG	SER	A	555	-13.003	3.936	12.781	1.00	41.21	O

ATOM	195	C	SER A 555	-11.378	6.287	13.071	1.00	43.51	C
ATOM	196	O	SER A 555	-11.393	7.015	12.078	1.00	44.45	O
ATOM	197	N	THR A 556	-10.273	5.683	13.498	1.00	42.04	N
ATOM	198	CA	THR A 556	-9.032	5.841	12.762	1.00	42.19	C
ATOM	199	CB	THR A 556	-7.881	5.035	13.406	1.00	42.32	C
ATOM	200	OG1	THR A 556	-7.516	5.646	14.651	1.00	42.04	O
ATOM	201	CG2	THR A 556	-6.659	5.006	12.499	1.00	41.12	C
ATOM	202	C	THR A 556	-9.293	5.367	11.337	1.00	42.74	C
ATOM	203	O	THR A 556	-8.766	5.928	10.378	1.00	42.87	O
ATOM	204	N	TRP A 557	-10.144	4.354	11.204	1.00	43.45	N
ATOM	205	CA	TRP A 557	-10.496	3.813	9.896	1.00	43.82	C
ATOM	206	CB	TRP A 557	-11.404	2.590	10.035	1.00	46.82	C
ATOM	207	CG	TRP A 557	-11.796	2.032	8.696	1.00	52.07	C
ATOM	208	CD2	TRP A 557	-12.973	2.357	7.936	1.00	53.78	C
ATOM	209	CE2	TRP A 557	-12.874	1.674	6.699	1.00	54.50	C
ATOM	210	CE3	TRP A 557	-14.099	3.162	8.177	1.00	55.10	C
ATOM	211	CD1	TRP A 557	-11.059	1.188	7.912	1.00	52.72	C
ATOM	212	NE1	TRP A 557	-11.697	0.970	6.714	1.00	53.41	N
ATOM	213	CZ2	TRP A 557	-13.860	1.770	5.701	1.00	55.60	C
ATOM	214	CZ3	TRP A 557	-15.082	3.260	7.183	1.00	56.65	C
ATOM	215	CH2	TRP A 557	-14.953	2.566	5.961	1.00	56.87	C
ATOM	216	C	TRP A 557	-11.217	4.843	9.027	1.00	42.69	C
ATOM	217	O	TRP A 557	-10.820	5.099	7.889	1.00	42.73	O
ATOM	218	N	ARG A 558	-12.289	5.422	9.558	1.00	40.54	N
ATOM	219	CA	ARG A 558	-13.050	6.398	8.798	1.00	39.82	C
ATOM	220	CB	ARG A 558	-14.308	6.803	9.567	1.00	41.39	C
ATOM	221	CG	ARG A 558	-14.995	5.631	10.230	1.00	44.29	C
ATOM	222	CD	ARG A 558	-16.424	5.936	10.670	1.00	47.40	C
ATOM	223	NE	ARG A 558	-16.569	7.212	11.370	1.00	48.53	N
ATOM	224	CZ	ARG A 558	-16.818	8.370	10.763	1.00	49.38	C
ATOM	225	NH1	ARG A 558	-16.944	8.410	9.443	1.00	49.04	N
ATOM	226	NH2	ARG A 558	-16.965	9.483	11.476	1.00	49.31	N
ATOM	227	C	ARG A 558	-12.219	7.629	8.457	1.00	37.44	C
ATOM	228	O	ARG A 558	-12.325	8.157	7.358	1.00	37.53	O
ATOM	229	N	ILE A 559	-11.395	8.084	9.397	1.00	35.98	N
ATOM	230	CA	ILE A 559	-10.550	9.256	9.176	1.00	34.05	C
ATOM	231	CB	ILE A 559	-9.832	9.695	10.468	1.00	33.19	C
ATOM	232	CG2	ILE A 559	-8.828	10.805	10.153	1.00	30.68	C
ATOM	233	CG1	ILE A 559	-10.867	10.148	11.503	1.00	31.75	C
ATOM	234	CD1	ILE A 559	-10.279	10.591	12.840	1.00	28.48	C
ATOM	235	C	ILE A 559	-9.497	9.019	8.093	1.00	33.57	C
ATOM	236	O	ILE A 559	-9.323	9.858	7.211	1.00	35.06	O
ATOM	237	N	MET A 560	-8.799	7.885	8.153	1.00	32.07	N
ATOM	238	CA	MET A 560	-7.775	7.568	7.151	1.00	31.33	C
ATOM	239	CB	MET A 560	-6.939	6.360	7.589	1.00	31.36	C
ATOM	240	CG	MET A 560	-6.173	6.558	8.888	1.00	32.80	C
ATOM	241	SD	MET A 560	-5.149	8.043	8.902	1.00	38.45	S
ATOM	242	CE	MET A 560	-4.032	7.699	7.487	1.00	31.35	C
ATOM	243	C	MET A 560	-8.392	7.282	5.782	1.00	29.65	C
ATOM	244	O	MET A 560	-7.797	7.570	4.745	1.00	30.30	O
ATOM	245	N	THR A 561	-9.584	6.703	5.780	1.00	28.64	N
ATOM	246	CA	THR A 561	-10.269	6.408	4.533	1.00	29.01	C
ATOM	247	CB	THR A 561	-11.524	5.552	4.789	1.00	29.96	C
ATOM	248	OG1	THR A 561	-11.130	4.292	5.354	1.00	31.59	O
ATOM	249	CG2	THR A 561	-12.276	5.307	3.489	1.00	30.13	C
ATOM	250	C	THR A 561	-10.672	7.731	3.876	1.00	29.38	C
ATOM	251	O	THR A 561	-10.548	7.907	2.661	1.00	28.77	O
ATOM	252	N	THR A 562	-11.149	8.663	4.695	1.00	28.92	N
ATOM	253	CA	THR A 562	-11.553	9.974	4.204	1.00	28.99	C
ATOM	254	CB	THR A 562	-12.219	10.831	5.319	1.00	30.42	C
ATOM	255	OG1	THR A 562	-13.428	10.196	5.758	1.00	28.64	O
ATOM	256	CG2	THR A 562	-12.547	12.230	4.794	1.00	29.72	C
ATOM	257	C	THR A 562	-10.323	10.708	3.691	1.00	27.30	C
ATOM	258	O	THR A 562	-10.322	11.245	2.584	1.00	27.79	O
ATOM	259	N	LEU A 563	-9.273	10.722	4.499	1.00	26.13	N
ATOM	260	CA	LEU A 563	-8.048	11.395	4.103	1.00	25.78	C

ATOM	261	CB	LEU A 563	-6.988	11.272	5.198	1.00	24.48	C
ATOM	262	CG	LEU A 563	-7.107	12.198	6.405	1.00	21.88	C
ATOM	263	CD1	LEU A 563	-5.930	11.971	7.336	1.00	20.16	C
ATOM	264	CD2	LEU A 563	-7.123	13.639	5.926	1.00	23.50	C
ATOM	265	C	LEU A 563	-7.511	10.823	2.798	1.00	26.34	C
ATOM	266	O	LEU A 563	-6.805	11.508	2.056	1.00	26.41	O
ATOM	267	N	ASN A 564	-7.847	9.573	2.504	1.00	26.91	N
ATOM	268	CA	ASN A 564	-7.353	8.983	1.272	1.00	28.34	C
ATOM	269	CB	ASN A 564	-7.551	7.472	1.288	1.00	30.39	C
ATOM	270	CG	ASN A 564	-6.687	6.775	0.254	1.00	33.88	C
ATOM	271	OD1	ASN A 564	-7.044	6.704	-0.930	1.00	31.52	O
ATOM	272	ND2	ASN A 564	-5.522	6.277	0.692	1.00	35.10	N
ATOM	273	C	ASN A 564	-8.022	9.603	0.047	1.00	27.58	C
ATOM	274	O	ASN A 564	-7.360	9.887	-0.958	1.00	26.59	O
ATOM	275	N	MET A 565	-9.329	9.832	0.143	1.00	28.68	N
ATOM	276	CA	MET A 565	-10.085	10.442	-0.950	1.00	29.27	C
ATOM	277	CB	MET A 565	-11.595	10.350	-0.697	1.00	33.18	C
ATOM	278	CG	MET A 565	-12.119	8.932	-0.554	1.00	39.91	C
ATOM	279	SD	MET A 565	-11.465	7.848	-1.856	1.00	49.04	S
ATOM	280	CE	MET A 565	-12.812	7.910	-3.109	1.00	46.85	C
ATOM	281	C	MET A 565	-9.705	11.908	-1.095	1.00	27.69	C
ATOM	282	O	MET A 565	-9.655	12.430	-2.206	1.00	28.50	O
ATOM	283	N	LEU A 566	-9.440	12.567	0.033	1.00	25.16	N
ATOM	284	CA	LEU A 566	-9.073	13.976	0.033	1.00	21.88	C
ATOM	285	CB	LEU A 566	-9.158	14.550	1.453	1.00	21.21	C
ATOM	286	CG	LEU A 566	-8.845	16.046	1.609	1.00	20.33	C
ATOM	287	CD1	LEU A 566	-9.831	16.868	0.789	1.00	17.51	C
ATOM	288	CD2	LEU A 566	-8.901	16.437	3.084	1.00	17.99	C
ATOM	289	C	LEU A 566	-7.674	14.179	-0.522	1.00	20.32	C
ATOM	290	O	LEU A 566	-7.433	15.120	-1.278	1.00	20.01	O
ATOM	291	N	GLY A 567	-6.752	13.298	-0.143	1.00	18.99	N
ATOM	292	CA	GLY A 567	-5.388	13.403	-0.634	1.00	18.66	C
ATOM	293	C	GLY A 567	-5.376	13.175	-2.132	1.00	19.42	C
ATOM	294	O	GLY A 567	-4.613	13.791	-2.877	1.00	19.90	O
ATOM	295	N	GLY A 568	-6.236	12.278	-2.586	1.00	18.70	N
ATOM	296	CA	GLY A 568	-6.299	12.030	-4.005	1.00	19.75	C
ATOM	297	C	GLY A 568	-6.747	13.290	-4.724	1.00	21.87	C
ATOM	298	O	GLY A 568	-6.142	13.693	-5.724	1.00	22.86	O
ATOM	299	N	ARG A 569	-7.806	13.922	-4.221	1.00	20.50	N
ATOM	300	CA	ARG A 569	-8.318	15.128	-4.850	1.00	20.17	C
ATOM	301	CB	ARG A 569	-9.660	15.516	-4.230	1.00	20.02	C
ATOM	302	CG	ARG A 569	-10.770	14.494	-4.480	1.00	20.32	C
ATOM	303	CD	ARG A 569	-11.931	14.685	-3.529	1.00	17.41	C
ATOM	304	NE	ARG A 569	-12.508	16.022	-3.614	1.00	20.04	N
ATOM	305	CZ	ARG A 569	-12.888	16.742	-2.556	1.00	20.90	C
ATOM	306	NH1	ARG A 569	-12.747	16.258	-1.323	1.00	17.50	N
ATOM	307	NH2	ARG A 569	-13.426	17.944	-2.732	1.00	20.21	N
ATOM	308	C	ARG A 569	-7.320	16.274	-4.728	1.00	22.52	C
ATOM	309	O	ARG A 569	-7.238	17.126	-5.610	1.00	25.40	O
ATOM	310	N	GLN A 570	-6.548	16.295	-3.647	1.00	22.17	N
ATOM	311	CA	GLN A 570	-5.569	17.364	-3.467	1.00	22.80	C
ATOM	312	CB	GLN A 570	-5.028	17.361	-2.045	1.00	21.90	C
ATOM	313	CG	GLN A 570	-6.081	17.673	-1.007	1.00	24.69	C
ATOM	314	CD	GLN A 570	-5.476	18.192	0.279	1.00	25.51	C
ATOM	315	OE1	GLN A 570	-6.191	18.570	1.209	1.00	26.69	O
ATOM	316	NE2	GLN A 570	-4.148	18.223	0.335	1.00	24.08	N
ATOM	317	C	GLN A 570	-4.411	17.282	-4.455	1.00	23.72	C
ATOM	318	O	GLN A 570	-3.875	18.318	-4.880	1.00	23.31	O
ATOM	319	N	VAL A 571	-4.021	16.055	-4.806	1.00	22.62	N
ATOM	320	CA	VAL A 571	-2.946	15.843	-5.763	1.00	22.08	C
ATOM	321	CB	VAL A 571	-2.661	14.324	-5.945	1.00	22.90	C
ATOM	322	CG1	VAL A 571	-1.680	14.101	-7.067	1.00	20.84	C
ATOM	323	CG2	VAL A 571	-2.094	13.744	-4.651	1.00	21.94	C
ATOM	324	C	VAL A 571	-3.394	16.477	-7.083	1.00	22.98	C
ATOM	325	O	VAL A 571	-2.697	17.334	-7.646	1.00	23.56	O
ATOM	326	N	ILE A 572	-4.570	16.077	-7.562	1.00	22.87	N

ATOM	327	CA	ILE	A	572	-5.109	16.631	-8.801	1.00	23.54	C
ATOM	328	CB	ILE	A	572	-6.571	16.164	-9.057	1.00	25.60	C
ATOM	329	CG2	ILE	A	572	-7.212	17.028	-10.138	1.00	23.10	C
ATOM	330	CG1	ILE	A	572	-6.598	14.698	-9.507	1.00	25.53	C
ATOM	331	CD1	ILE	A	572	-5.914	13.765	-8.563	1.00	28.80	C
ATOM	332	C	ILE	A	572	-5.091	18.157	-8.756	1.00	23.17	C
ATOM	333	O	ILE	A	572	-4.760	18.810	-9.740	1.00	26.20	O
ATOM	334	N	ALA	A	573	-5.444	18.731	-7.614	1.00	21.88	N
ATOM	335	CA	ALA	A	573	-5.445	20.179	-7.484	1.00	20.37	C
ATOM	336	CB	ALA	A	573	-6.173	20.594	-6.216	1.00	18.79	C
ATOM	337	C	ALA	A	573	-4.018	20.723	-7.477	1.00	20.64	C
ATOM	338	O	ALA	A	573	-3.780	21.857	-7.885	1.00	20.41	O
ATOM	339	N	ALA	A	574	-3.069	19.918	-7.009	1.00	20.63	N
ATOM	340	CA	ALA	A	574	-1.674	20.347	-6.976	1.00	22.06	C
ATOM	341	CB	ALA	A	574	-0.859	19.428	-6.075	1.00	21.71	C
ATOM	342	C	ALA	A	574	-1.096	20.341	-8.390	1.00	22.27	C
ATOM	343	O	ALA	A	574	-0.229	21.153	-8.729	1.00	22.45	O
ATOM	344	N	VAL	A	575	-1.580	19.409	-9.203	1.00	21.27	N
ATOM	345	CA	VAL	A	575	-1.145	19.273	-10.583	1.00	22.34	C
ATOM	346	CB	VAL	A	575	-1.695	17.950	-11.210	1.00	24.69	C
ATOM	347	CG1	VAL	A	575	-1.378	17.899	-12.686	1.00	21.88	C
ATOM	348	CG2	VAL	A	575	-1.092	16.708	-10.484	1.00	24.59	C
ATOM	349	C	VAL	A	575	-1.697	20.464	-11.360	1.00	25.30	C
ATOM	350	O	VAL	A	575	-0.996	21.094	-12.163	1.00	24.89	O
ATOM	351	N	LYS	A	576	-2.964	20.777	-11.108	1.00	26.15	N
ATOM	352	CA	LYS	A	576	-3.628	21.883	-11.778	1.00	26.08	C
ATOM	353	CB	LYS	A	576	-5.100	21.892	-11.362	1.00	29.82	C
ATOM	354	CG	LYS	A	576	-5.936	23.016	-11.932	1.00	35.73	C
ATOM	355	CD	LYS	A	576	-6.131	22.864	-13.430	1.00	41.72	C
ATOM	356	CE	LYS	A	576	-7.184	23.840	-13.934	1.00	43.06	C
ATOM	357	NZ	LYS	A	576	-8.423	23.729	-13.105	1.00	44.70	N
ATOM	358	C	LYS	A	576	-2.927	23.198	-11.414	1.00	25.77	C
ATOM	359	O	LYS	A	576	-2.708	24.068	-12.268	1.00	26.93	O
ATOM	360	N	TRP	A	577	-2.561	23.326	-10.142	1.00	23.23	N
ATOM	361	CA	TRP	A	577	-1.875	24.510	-9.637	1.00	21.37	C
ATOM	362	CB	TRP	A	577	-1.746	24.411	-8.120	1.00	18.79	C
ATOM	363	CG	TRP	A	577	-0.719	25.321	-7.537	1.00	19.34	C
ATOM	364	CD2	TRP	A	577	0.625	24.968	-7.165	1.00	17.94	C
ATOM	365	CE2	TRP	A	577	1.243	26.142	-6.671	1.00	18.46	C
ATOM	366	CE3	TRP	A	577	1.366	23.779	-7.206	1.00	15.69	C
ATOM	367	CD1	TRP	A	577	-0.856	26.657	-7.264	1.00	18.48	C
ATOM	368	NE1	TRP	A	577	0.320	27.157	-6.742	1.00	17.97	N
ATOM	369	CZ2	TRP	A	577	2.573	26.156	-6.218	1.00	16.37	C
ATOM	370	CZ3	TRP	A	577	2.686	23.796	-6.762	1.00	17.86	C
ATOM	371	CH2	TRP	A	577	3.274	24.976	-6.275	1.00	15.83	C
ATOM	372	C	TRP	A	577	-0.491	24.626	-10.270	1.00	23.06	C
ATOM	373	O	TRP	A	577	-0.118	25.683	-10.805	1.00	21.69	O
ATOM	374	N	ALA	A	578	0.264	23.531	-10.206	1.00	24.00	N
ATOM	375	CA	ALA	A	578	1.611	23.482	-10.762	1.00	24.36	C
ATOM	376	CB	ALA	A	578	2.189	22.096	-10.571	1.00	23.59	C
ATOM	377	C	ALA	A	578	1.622	23.867	-12.245	1.00	26.21	C
ATOM	378	O	ALA	A	578	2.414	24.720	-12.667	1.00	24.47	O
ATOM	379	N	LYS	A	579	0.734	23.239	-13.020	1.00	28.56	N
ATOM	380	CA	LYS	A	579	0.605	23.491	-14.459	1.00	29.95	C
ATOM	381	CB	LYS	A	579	-0.625	22.769	-15.029	1.00	32.43	C
ATOM	382	CG	LYS	A	579	-0.514	21.242	-15.148	1.00	35.06	C
ATOM	383	CD	LYS	A	579	0.473	20.833	-16.232	1.00	38.17	C
ATOM	384	CE	LYS	A	579	0.491	19.323	-16.442	1.00	40.07	C
ATOM	385	NZ	LYS	A	579	-0.806	18.793	-16.968	1.00	40.93	N
ATOM	386	C	LYS	A	579	0.485	24.974	-14.789	1.00	30.72	C
ATOM	387	O	LYS	A	579	0.934	25.412	-15.839	1.00	32.12	O
ATOM	388	N	ALA	A	580	-0.115	25.751	-13.895	1.00	30.95	N
ATOM	389	CA	ALA	A	580	-0.279	27.181	-14.144	1.00	29.86	C
ATOM	390	CB	ALA	A	580	-1.630	27.656	-13.602	1.00	28.78	C
ATOM	391	C	ALA	A	580	0.842	28.045	-13.573	1.00	29.74	C
ATOM	392	O	ALA	A	580	0.747	29.270	-13.596	1.00	30.94	O

ATOM	393	N	ILE	A	581	1.901	27.424	-13.063	1.00	28.55	N
ATOM	394	CA	ILE	A	581	3.008	28.195	-12.508	1.00	27.50	C
ATOM	395	CB	ILE	A	581	3.940	27.339	-11.606	1.00	27.31	C
ATOM	396	CG2	ILE	A	581	5.174	28.161	-11.227	1.00	23.78	C
ATOM	397	CG1	ILE	A	581	3.219	26.881	-10.331	1.00	25.65	C
ATOM	398	CD1	ILE	A	581	3.045	27.960	-9.288	1.00	26.32	C
ATOM	399	C	ILE	A	581	3.882	28.793	-13.613	1.00	29.17	O
ATOM	400	O	ILE	A	581	4.497	28.070	-14.402	1.00	28.76	N
ATOM	401	N	PRO	A	582	3.947	30.128	-13.680	1.00	29.58	C
ATOM	402	CD	PRO	A	582	3.314	31.083	-12.751	1.00	28.98	C
ATOM	403	CA	PRO	A	582	4.757	30.820	-14.687	1.00	29.20	C
ATOM	404	CB	PRO	A	582	4.789	32.253	-14.168	1.00	29.68	C
ATOM	405	CG	PRO	A	582	3.458	32.391	-13.481	1.00	29.84	C
ATOM	406	C	PRO	A	582	6.149	30.197	-14.724	1.00	29.77	O
ATOM	407	O	PRO	A	582	6.721	29.900	-13.675	1.00	28.16	N
ATOM	408	N	GLY	A	583	6.691	29.994	-15.923	1.00	31.70	C
ATOM	409	CA	GLY	A	583	8.017	29.398	-16.045	1.00	33.62	C
ATOM	410	C	GLY	A	583	7.981	27.877	-16.047	1.00	35.09	O
ATOM	411	O	GLY	A	583	8.350	27.229	-17.030	1.00	36.64	N
ATOM	412	N	PHE	A	584	7.540	27.310	-14.929	1.00	35.06	C
ATOM	413	CA	PHE	A	584	7.416	25.870	-14.771	1.00	34.81	C
ATOM	414	CB	PHE	A	584	6.800	25.563	-13.405	1.00	33.94	C
ATOM	415	CG	PHE	A	584	6.433	24.118	-13.200	1.00	31.93	C
ATOM	416	CD1	PHE	A	584	7.342	23.224	-12.643	1.00	31.47	C
ATOM	417	CD2	PHE	A	584	5.156	23.666	-13.516	1.00	31.80	C
ATOM	418	CE1	PHE	A	584	6.982	21.901	-12.393	1.00	31.19	C
ATOM	419	CE2	PHE	A	584	4.784	22.350	-13.274	1.00	30.92	C
ATOM	420	CZ	PHE	A	584	5.697	21.464	-12.709	1.00	31.95	C
ATOM	421	C	PHE	A	584	6.528	25.309	-15.875	1.00	35.45	O
ATOM	422	O	PHE	A	584	6.824	24.260	-16.436	1.00	35.68	N
ATOM	423	N	ARG	A	585	5.446	26.016	-16.188	1.00	36.88	C
ATOM	424	CA	ARG	A	585	4.501	25.569	-17.219	1.00	39.05	C
ATOM	425	CB	ARG	A	585	3.322	26.549	-17.319	1.00	40.69	C
ATOM	426	CG	ARG	A	585	3.703	27.999	-17.630	1.00	44.66	C
ATOM	427	CD	ARG	A	585	2.457	28.872	-17.760	1.00	47.75	N
ATOM	428	NE	ARG	A	585	1.557	28.385	-18.810	1.00	52.24	C
ATOM	429	CZ	ARG	A	585	0.362	28.904	-19.085	1.00	52.79	N
ATOM	430	NH1	ARG	A	585	-0.096	29.936	-18.388	1.00	53.76	N
ATOM	431	NH2	ARG	A	585	-0.379	28.386	-20.056	1.00	53.73	C
ATOM	432	C	ARG	A	585	5.112	25.371	-18.614	1.00	38.66	O
ATOM	433	O	ARG	A	585	4.563	24.637	-19.448	1.00	38.04	N
ATOM	434	N	ASN	A	586	6.250	26.017	-18.855	1.00	38.54	C
ATOM	435	CA	ASN	A	586	6.936	25.948	-20.142	1.00	38.28	C
ATOM	436	CB	ASN	A	586	7.640	27.279	-20.425	1.00	38.83	C
ATOM	437	CG	ASN	A	586	6.664	28.448	-20.564	1.00	39.20	O
ATOM	438	OD1	ASN	A	586	7.000	29.585	-20.223	1.00	39.24	N
ATOM	439	ND2	ASN	A	586	5.461	28.175	-21.079	1.00	36.46	C
ATOM	440	C	ASN	A	586	7.949	24.814	-20.213	1.00	38.85	O
ATOM	441	O	ASN	A	586	8.586	24.609	-21.247	1.00	40.05	N
ATOM	442	N	LEU	A	587	8.120	24.102	-19.104	1.00	38.19	C
ATOM	443	CA	LEU	A	587	9.037	22.974	-19.053	1.00	35.53	C
ATOM	444	CB	LEU	A	587	9.343	22.594	-17.605	1.00	36.50	C
ATOM	445	CG	LEU	A	587	10.244	23.527	-16.788	1.00	37.76	C
ATOM	446	CD1	LEU	A	587	10.247	23.077	-15.338	1.00	36.40	C
ATOM	447	CD2	LEU	A	587	11.663	23.513	-17.353	1.00	36.25	C
ATOM	448	C	LEU	A	587	8.360	21.801	-19.748	1.00	35.11	O
ATOM	449	O	LEU	A	587	7.130	21.725	-19.812	1.00	33.16	N
ATOM	450	N	HIS	A	588	9.167	20.889	-20.275	1.00	33.14	C
ATOM	451	CA	HIS	A	588	8.642	19.720	-20.957	1.00	30.67	C
ATOM	452	CB	HIS	A	588	9.803	18.840	-21.435	1.00	31.28	C
ATOM	453	CG	HIS	A	588	9.389	17.748	-22.371	1.00	31.81	C
ATOM	454	CD2	HIS	A	588	9.385	17.690	-23.725	1.00	30.94	N
ATOM	455	ND1	HIS	A	588	8.870	16.548	-21.934	1.00	31.37	C
ATOM	456	CE1	HIS	A	588	8.564	15.798	-22.979	1.00	32.18	N
ATOM	457	NE2	HIS	A	588	8.866	16.468	-24.077	1.00	32.69	C
ATOM	458	C	HIS	A	588	7.766	18.957	-19.972	1.00	29.79	C

ATOM	459	O	HIS	A	588	8.086	18.893	-18.785	1.00	30.89	O
ATOM	460	N	LEU	A	589	6.668	18.381	-20.457	1.00	28.76	N
ATOM	461	CA	LEU	A	589	5.761	17.628	-19.592	1.00	27.43	C
ATOM	462	CB	LEU	A	589	4.716	16.879	-20.413	1.00	28.13	C
ATOM	463	CG	LEU	A	589	3.290	17.434	-20.343	1.00	29.92	C
ATOM	464	CD1	LEU	A	589	2.766	17.388	-18.919	1.00	29.73	C
ATOM	465	CD2	LEU	A	589	3.288	18.857	-20.854	1.00	32.32	C
ATOM	466	C	LEU	A	589	6.487	16.637	-18.699	1.00	26.92	C
ATOM	467	O	LEU	A	589	6.206	16.555	-17.516	1.00	26.21	O
ATOM	468	N	ASP	A	590	7.417	15.878	-19.264	1.00	27.79	N
ATOM	469	CA	ASP	A	590	8.163	14.912	-18.468	1.00	28.63	C
ATOM	470	CB	ASP	A	590	9.227	14.205	-19.310	1.00	28.13	C
ATOM	471	CG	ASP	A	590	8.645	13.127	-20.190	1.00	31.35	C
ATOM	472	OD1	ASP	A	590	7.678	12.452	-19.751	1.00	33.05	O
ATOM	473	OD2	ASP	A	590	9.167	12.945	-21.312	1.00	32.29	O
ATOM	474	C	ASP	A	590	8.830	15.541	-17.253	1.00	28.09	C
ATOM	475	O	ASP	A	590	8.856	14.938	-16.182	1.00	29.48	O
ATOM	476	N	ASP	A	591	9.374	16.745	-17.418	1.00	26.75	N
ATOM	477	CA	ASP	A	591	10.039	17.433	-16.313	1.00	26.10	C
ATOM	478	CB	ASP	A	591	10.879	18.601	-16.832	1.00	25.04	C
ATOM	479	CG	ASP	A	591	12.197	18.159	-17.437	1.00	25.45	C
ATOM	480	OD1	ASP	A	591	12.464	16.936	-17.524	1.00	25.61	O
ATOM	481	OD2	ASP	A	591	12.974	19.056	-17.826	1.00	25.71	O
ATOM	482	C	ASP	A	591	9.036	17.951	-15.284	1.00	26.07	C
ATOM	483	O	ASP	A	591	9.348	18.066	-14.101	1.00	25.75	O
ATOM	484	N	GLN	A	592	7.837	18.284	-15.745	1.00	25.37	N
ATOM	485	CA	GLN	A	592	6.803	18.776	-14.855	1.00	24.97	C
ATOM	486	CB	GLN	A	592	5.658	19.382	-15.663	1.00	24.27	C
ATOM	487	CG	GLN	A	592	6.028	20.659	-16.377	1.00	25.93	C
ATOM	488	CD	GLN	A	592	4.841	21.300	-17.073	1.00	26.52	C
ATOM	489	OE1	GLN	A	592	3.791	21.484	-16.479	1.00	29.15	O
ATOM	490	NE2	GLN	A	592	5.013	21.654	-18.335	1.00	27.88	N
ATOM	491	C	GLN	A	592	6.285	17.629	-13.993	1.00	25.20	C
ATOM	492	O	GLN	A	592	6.115	17.775	-12.772	1.00	26.51	O
ATOM	493	N	MET	A	593	6.047	16.489	-14.636	1.00	23.72	N
ATOM	494	CA	MET	A	593	5.548	15.296	-13.962	1.00	24.08	C
ATOM	495	CB	MET	A	593	5.202	14.222	-14.992	1.00	23.80	C
ATOM	496	CG	MET	A	593	4.003	14.570	-15.849	1.00	24.95	C
ATOM	497	SD	MET	A	593	2.531	14.931	-14.838	1.00	29.41	S
ATOM	498	CE	MET	A	593	2.470	16.722	-14.955	1.00	28.41	C
ATOM	499	C	MET	A	593	6.558	14.747	-12.961	1.00	24.06	C
ATOM	500	O	MET	A	593	6.181	14.157	-11.947	1.00	22.92	O
ATOM	501	N	THR	A	594	7.841	14.950	-13.259	1.00	24.52	N
ATOM	502	CA	THR	A	594	8.931	14.495	-12.401	1.00	25.08	C
ATOM	503	CB	THR	A	594	10.298	14.606	-13.132	1.00	26.55	C
ATOM	504	OG1	THR	A	594	10.320	13.685	-14.226	1.00	26.87	O
ATOM	505	CG2	THR	A	594	11.468	14.302	-12.177	1.00	24.40	C
ATOM	506	C	THR	A	594	8.979	15.323	-11.120	1.00	25.46	C
ATOM	507	O	THR	A	594	8.960	14.772	-10.020	1.00	25.68	O
ATOM	508	N	LEU	A	595	9.036	16.644	-11.272	1.00	24.93	N
ATOM	509	CA	LEU	A	595	9.081	17.557	-10.134	1.00	25.45	C
ATOM	510	CB	LEU	A	595	9.168	19.007	-10.630	1.00	22.72	C
ATOM	511	CG	LEU	A	595	10.338	19.324	-11.570	1.00	19.93	C
ATOM	512	CD1	LEU	A	595	10.218	20.745	-12.133	1.00	17.88	C
ATOM	513	CD2	LEU	A	595	11.630	19.144	-10.814	1.00	15.94	C
ATOM	514	C	LEU	A	595	7.848	17.384	-9.235	1.00	26.07	C
ATOM	515	O	LEU	A	595	7.949	17.475	-8.013	1.00	27.68	O
ATOM	516	N	LEU	A	596	6.690	17.148	-9.846	1.00	25.55	N
ATOM	517	CA	LEU	A	596	5.454	16.947	-9.094	1.00	25.56	C
ATOM	518	CB	LEU	A	596	4.249	17.053	-10.031	1.00	25.22	C
ATOM	519	CG	LEU	A	596	3.845	18.474	-10.433	1.00	26.08	C
ATOM	520	CD1	LEU	A	596	2.821	18.427	-11.568	1.00	25.36	C
ATOM	521	CD2	LEU	A	596	3.276	19.204	-9.223	1.00	24.95	C
ATOM	522	C	LEU	A	596	5.484	15.574	-8.411	1.00	25.76	C
ATOM	523	O	LEU	A	596	4.963	15.392	-7.312	1.00	23.66	O
ATOM	524	N	GLN	A	597	6.098	14.604	-9.072	1.00	26.73	N

ATOM	525	CA	GLN	A	597	6.212	13.274	-8.491	1.00	27.83	C
ATOM	526	CB	GLN	A	597	6.885	12.319	-9.473	1.00	28.94	C
ATOM	527	CG	GLN	A	597	6.850	10.867	-9.039	1.00	33.49	C
ATOM	528	CD	GLN	A	597	7.781	10.012	-9.861	1.00	36.00	C
ATOM	529	OE1	GLN	A	597	7.829	10.129	-11.087	1.00	38.65	O
ATOM	530	NE2	GLN	A	597	8.525	9.140	-9.197	1.00	38.09	N
ATOM	531	C	GLN	A	597	7.061	13.362	-7.220	1.00	25.65	C
ATOM	532	O	GLN	A	597	6.809	12.661	-6.245	1.00	24.70	O
ATOM	533	N	TYR	A	598	8.059	14.237	-7.241	1.00	24.14	N
ATOM	534	CA	TYR	A	598	8.961	14.412	-6.106	1.00	24.05	C
ATOM	535	CB	TYR	A	598	10.347	14.875	-6.577	1.00	24.63	C
ATOM	536	CG	TYR	A	598	11.086	13.900	-7.447	1.00	26.03	C
ATOM	537	CD1	TYR	A	598	12.243	14.284	-8.129	1.00	27.95	C
ATOM	538	CE1	TYR	A	598	12.926	13.377	-8.955	1.00	28.73	C
ATOM	539	CD2	TYR	A	598	10.628	12.592	-7.601	1.00	27.21	C
ATOM	540	CE2	TYR	A	598	11.293	11.691	-8.413	1.00	26.80	C
ATOM	541	CZ	TYR	A	598	12.434	12.084	-9.088	1.00	29.01	C
ATOM	542	OH	TYR	A	598	13.054	11.174	-9.910	1.00	33.28	O
ATOM	543	C	TYR	A	598	8.489	15.420	-5.077	1.00	22.65	C
ATOM	544	O	TYR	A	598	9.074	15.509	-4.006	1.00	23.56	O
ATOM	545	N	SER	A	599	7.440	16.174	-5.379	1.00	20.97	N
ATOM	546	CA	SER	A	599	7.022	17.191	-4.435	1.00	19.00	C
ATOM	547	CB	SER	A	599	7.436	18.550	-4.985	1.00	20.03	C
ATOM	548	OG	SER	A	599	6.588	18.912	-6.059	1.00	19.53	C
ATOM	549	C	SER	A	599	5.561	17.267	-4.000	1.00	19.15	C
ATOM	550	O	SER	A	599	5.242	18.088	-3.131	1.00	18.38	O
ATOM	551	N	TRP	A	600	4.671	16.443	-4.557	1.00	15.40	N
ATOM	552	CA	TRP	A	600	3.275	16.560	-4.151	1.00	17.13	C
ATOM	553	CB	TRP	A	600	2.376	15.562	-4.897	1.00	17.24	C
ATOM	554	CG	TRP	A	600	2.623	14.118	-4.605	1.00	18.87	C
ATOM	555	CD2	TRP	A	600	2.079	13.360	-3.519	1.00	19.51	C
ATOM	556	CE2	TRP	A	600	2.561	12.041	-3.649	1.00	20.31	C
ATOM	557	CE3	TRP	A	600	1.225	13.665	-2.450	1.00	20.20	C
ATOM	558	CD1	TRP	A	600	3.395	13.255	-5.326	1.00	16.67	C
ATOM	559	NE1	TRP	A	600	3.364	12.007	-4.758	1.00	19.08	N
ATOM	560	CZ2	TRP	A	600	2.217	11.021	-2.744	1.00	22.72	C
ATOM	561	CZ3	TRP	A	600	0.882	12.653	-1.552	1.00	18.94	C
ATOM	562	CH2	TRP	A	600	1.378	11.348	-1.705	1.00	20.70	C
ATOM	563	C	TRP	A	600	3.047	16.450	-2.633	1.00	19.20	C
ATOM	564	O	TRP	A	600	2.249	17.212	-2.063	1.00	18.82	O
ATOM	565	N	MET	A	601	3.746	15.525	-1.977	1.00	17.50	N
ATOM	566	CA	MET	A	601	3.598	15.354	-0.532	1.00	17.71	C
ATOM	567	CB	MET	A	601	4.410	14.140	-0.051	1.00	16.60	C
ATOM	568	CG	MET	A	601	4.215	13.788	1.415	1.00	17.40	C
ATOM	569	SD	MET	A	601	2.492	13.436	1.886	1.00	19.62	S
ATOM	570	CE	MET	A	601	2.394	11.675	1.631	1.00	16.85	C
ATOM	571	C	MET	A	601	4.061	16.624	0.189	1.00	17.89	C
ATOM	572	O	MET	A	601	3.368	17.148	1.071	1.00	17.68	O
ATOM	573	N	SER	A	602	5.229	17.118	-0.207	1.00	16.80	N
ATOM	574	CA	SER	A	602	5.806	18.323	0.376	1.00	15.49	C
ATOM	575	CB	SER	A	602	7.131	18.636	-0.330	1.00	17.10	C
ATOM	576	OG	SER	A	602	7.847	19.680	0.303	1.00	20.10	O
ATOM	577	C	SER	A	602	4.834	19.509	0.250	1.00	15.33	C
ATOM	578	O	SER	A	602	4.579	20.226	1.221	1.00	16.43	O
ATOM	579	N	LEU	A	603	4.288	19.708	-0.943	1.00	15.45	N
ATOM	580	CA	LEU	A	603	3.347	20.798	-1.199	1.00	14.55	C
ATOM	581	CB	LEU	A	603	2.985	20.842	-2.688	1.00	14.71	C
ATOM	582	CG	LEU	A	603	4.113	21.118	-3.689	1.00	12.50	C
ATOM	583	CD1	LEU	A	603	3.637	20.799	-5.109	1.00	15.59	C
ATOM	584	CD2	LEU	A	603	4.556	22.569	-3.590	1.00	8.56	C
ATOM	585	C	LEU	A	603	2.068	20.640	-0.370	1.00	16.48	C
ATOM	586	O	LEU	A	603	1.571	21.615	0.212	1.00	16.14	O
ATOM	587	N	MET	A	604	1.534	19.420	-0.308	1.00	16.26	N
ATOM	588	CA	MET	A	604	0.312	19.193	0.456	1.00	18.92	C
ATOM	589	CB	MET	A	604	-0.275	17.815	0.137	1.00	18.51	C
ATOM	590	CG	MET	A	604	-1.153	17.839	-1.113	1.00	21.33	C

ATOM	591	SD	MET	A	604	-1.346	16.258	-1.969	1.00	24.51	S
ATOM	592	CE	MET	A	604	-2.048	15.250	-0.626	1.00	20.51	C
ATOM	593	C	MET	A	604	0.512	19.371	1.959	1.00	19.09	C
ATOM	594	O	MET	A	604	-0.376	19.884	2.647	1.00	17.52	O
ATOM	595	N	ALA	A	605	1.681	18.966	2.455	1.00	18.28	N
ATOM	596	CA	ALA	A	605	2.009	19.107	3.875	1.00	16.81	C
ATOM	597	CB	ALA	A	605	3.265	18.332	4.206	1.00	14.60	C
ATOM	598	C	ALA	A	605	2.219	20.579	4.220	1.00	17.64	C
ATOM	599	O	ALA	A	605	1.866	21.031	5.320	1.00	15.68	O
ATOM	600	N	PHE	A	606	2.802	21.316	3.271	1.00	17.60	N
ATOM	601	CA	PHE	A	606	3.076	22.732	3.460	1.00	14.90	C
ATOM	602	CB	PHE	A	606	3.965	23.259	2.340	1.00	14.99	C
ATOM	603	CG	PHE	A	606	4.654	24.542	2.685	1.00	15.85	C
ATOM	604	CD1	PHE	A	606	5.607	24.573	3.698	1.00	15.60	C
ATOM	605	CD2	PHE	A	606	4.319	25.732	2.041	1.00	17.41	C
ATOM	606	CE1	PHE	A	606	6.215	25.764	4.070	1.00	13.51	C
ATOM	607	CE2	PHE	A	606	4.927	26.941	2.411	1.00	14.18	C
ATOM	608	CZ	PHE	A	606	5.872	26.951	3.424	1.00	14.61	C
ATOM	609	C	PHE	A	606	1.787	23.557	3.521	1.00	14.99	C
ATOM	610	O	PHE	A	606	1.651	24.429	4.379	1.00	16.12	O
ATOM	611	N	ALA	A	607	0.850	23.288	2.609	1.00	14.14	N
ATOM	612	CA	ALA	A	607	-0.433	24.003	2.572	1.00	12.28	C
ATOM	613	CB	ALA	A	607	-1.251	23.581	1.339	1.00	7.48	C
ATOM	614	C	ALA	A	607	-1.217	23.692	3.841	1.00	12.83	C
ATOM	615	O	ALA	A	607	-1.844	24.583	4.436	1.00	12.84	O
ATOM	616	N	LEU	A	608	-1.196	22.417	4.236	1.00	13.10	N
ATOM	617	CA	LEU	A	608	-1.883	21.968	5.435	1.00	13.47	C
ATOM	618	CB	LEU	A	608	-1.674	20.464	5.635	1.00	13.37	C
ATOM	619	CG	LEU	A	608	-2.059	19.827	6.978	1.00	12.59	C
ATOM	620	CD1	LEU	A	608	-3.505	20.155	7.304	1.00	12.66	C
ATOM	621	CD2	LEU	A	608	-1.840	18.315	6.913	1.00	7.59	C
ATOM	622	C	LEU	A	608	-1.299	22.761	6.605	1.00	15.21	C
ATOM	623	O	LEU	A	608	-2.042	23.288	7.440	1.00	15.56	O
ATOM	624	N	GLY	A	609	0.031	22.864	6.630	1.00	14.81	N
ATOM	625	CA	GLY	A	609	0.706	23.609	7.673	1.00	14.53	C
ATOM	626	C	GLY	A	609	0.208	25.042	7.678	1.00	18.21	C
ATOM	627	O	GLY	A	609	-0.016	25.640	8.743	1.00	16.57	O
ATOM	628	N	TRP	A	610	0.025	25.608	6.485	1.00	18.92	N
ATOM	629	CA	TRP	A	610	-0.456	26.975	6.391	1.00	19.51	C
ATOM	630	CB	TRP	A	610	-0.317	27.500	4.969	1.00	22.20	C
ATOM	631	CG	TRP	A	610	-0.820	28.904	4.822	1.00	26.46	C
ATOM	632	CD2	TRP	A	610	-0.146	30.110	5.229	1.00	28.37	C
ATOM	633	CE2	TRP	A	610	-1.003	31.194	4.918	1.00	28.78	C
ATOM	634	CE3	TRP	A	610	1.096	30.379	5.824	1.00	27.32	C
ATOM	635	CD1	TRP	A	610	-2.020	29.294	4.299	1.00	26.45	C
ATOM	636	NE1	TRP	A	610	-2.137	30.668	4.354	1.00	29.69	N
ATOM	637	CZ2	TRP	A	610	-0.656	32.526	5.178	1.00	27.49	C
ATOM	638	CZ3	TRP	A	610	1.441	31.706	6.082	1.00	28.88	C
ATOM	639	CH2	TRP	A	610	0.564	32.762	5.758	1.00	28.83	C
ATOM	640	C	TRP	A	610	-1.905	27.094	6.865	1.00	19.11	C
ATOM	641	O	TRP	A	610	-2.256	28.052	7.547	1.00	19.32	O
ATOM	642	N	ARG	A	611	-2.750	26.128	6.524	1.00	18.74	N
ATOM	643	CA	ARG	A	611	-4.127	26.204	6.990	1.00	19.68	C
ATOM	644	CB	ARG	A	611	-4.989	25.075	6.396	1.00	19.92	C
ATOM	645	CG	ARG	A	611	-5.292	25.261	4.901	1.00	17.15	C
ATOM	646	CD	ARG	A	611	-6.378	24.315	4.394	1.00	14.12	C
ATOM	647	NE	ARG	A	611	-6.043	22.898	4.533	1.00	17.44	N
ATOM	648	CZ	ARG	A	611	-5.271	22.208	3.692	1.00	19.79	C
ATOM	649	NH1	ARG	A	611	-4.730	22.786	2.623	1.00	21.94	N
ATOM	650	NH2	ARG	A	611	-5.050	20.919	3.911	1.00	20.74	N
ATOM	651	C	ARG	A	611	-4.151	26.146	8.517	1.00	19.29	C
ATOM	652	O	ARG	A	611	-4.703	27.034	9.148	1.00	17.58	O
ATOM	653	N	SER	A	612	-3.528	25.116	9.092	1.00	20.00	N
ATOM	654	CA	SER	A	612	-3.476	24.920	10.541	1.00	22.03	C
ATOM	655	CB	SER	A	612	-2.477	23.808	10.889	1.00	20.76	C
ATOM	656	OG	SER	A	612	-2.900	22.565	10.354	1.00	19.33	O

ATOM	657	C	SER A 612	-3.096	26.190	11.289	1.00	25.12	C
ATOM	658	O	SER A 612	-3.745	26.568	12.267	1.00	27.06	O
ATOM	659	N	TYR A 613	-2.034	26.832	10.818	1.00	27.13	N
ATOM	660	CA	TYR A 613	-1.527	28.067	11.390	1.00	29.28	C
ATOM	661	CB	TYR A 613	-0.214	28.420	10.707	1.00	30.39	C
ATOM	662	CG	TYR A 613	0.205	29.867	10.800	1.00	31.94	C
ATOM	663	CD1	TYR A 613	0.277	30.527	12.028	1.00	33.61	C
ATOM	664	CE1	TYR A 613	0.761	31.842	12.113	1.00	35.43	C
ATOM	665	CD2	TYR A 613	0.616	30.555	9.660	1.00	31.78	C
ATOM	666	CE2	TYR A 613	1.098	31.856	9.731	1.00	33.01	C
ATOM	667	CZ	TYR A 613	1.172	32.493	10.953	1.00	34.95	C
ATOM	668	OH	TYR A 613	1.676	33.772	11.000	1.00	38.65	O
ATOM	669	C	TYR A 613	-2.520	29.213	11.235	1.00	31.91	C
ATOM	670	O	TYR A 613	-2.785	29.942	12.185	1.00	33.31	O
ATOM	671	N	ARG A 614	-3.061	29.376	10.036	1.00	33.98	N
ATOM	672	CA	ARG A 614	-4.023	30.438	9.781	1.00	36.74	C
ATOM	673	CB	ARG A 614	-4.305	30.540	8.279	1.00	39.03	C
ATOM	674	CG	ARG A 614	-3.685	31.729	7.576	1.00	43.69	C
ATOM	675	CD	ARG A 614	-2.895	32.605	8.519	1.00	47.27	C
ATOM	676	NE	ARG A 614	-2.888	33.987	8.060	1.00	52.81	N
ATOM	677	CZ	ARG A 614	-2.238	34.971	8.673	1.00	56.27	C
ATOM	678	NH1	ARG A 614	-1.538	34.719	9.776	1.00	56.73	N
ATOM	679	NH2	ARG A 614	-2.291	36.210	8.187	1.00	57.85	N
ATOM	680	C	ARG A 614	-5.350	30.250	10.519	1.00	37.83	C
ATOM	681	O	ARG A 614	-5.895	31.201	11.075	1.00	38.44	O
ATOM	682	N	GLN A 615	-5.871	29.026	10.518	1.00	37.95	N
ATOM	683	CA	GLN A 615	-7.155	28.739	11.154	1.00	37.73	C
ATOM	684	CB	GLN A 615	-7.758	27.446	10.586	1.00	37.47	C
ATOM	685	CG	GLN A 615	-7.885	27.416	9.071	1.00	39.17	C
ATOM	686	CD	GLN A 615	-8.691	28.584	8.511	1.00	41.61	O
ATOM	687	OE1	GLN A 615	-9.883	28.728	8.788	1.00	42.90	N
ATOM	688	NE2	GLN A 615	-8.037	29.424	7.718	1.00	41.96	C
ATOM	689	C	GLN A 615	-7.132	28.635	12.674	1.00	37.35	O
ATOM	690	O	GLN A 615	-7.879	29.334	13.358	1.00	37.67	N
ATOM	691	N	SER A 616	-6.271	27.767	13.197	1.00	37.18	C
ATOM	692	CA	SER A 616	-6.176	27.536	14.639	1.00	36.04	C
ATOM	693	CB	SER A 616	-6.396	26.053	14.928	1.00	35.20	O
ATOM	694	OG	SER A 616	-5.371	25.274	14.325	1.00	31.48	C
ATOM	695	C	SER A 616	-4.848	27.945	15.258	1.00	36.93	O
ATOM	696	O	SER A 616	-4.395	27.313	16.211	1.00	37.77	N
ATOM	697	N	SER A 617	-4.221	28.985	14.718	1.00	37.08	C
ATOM	698	CA	SER A 617	-2.938	29.461	15.229	1.00	36.65	C
ATOM	699	CB	SER A 617	-3.142	30.229	16.540	1.00	36.79	O
ATOM	700	OG	SER A 617	-3.976	31.356	16.344	1.00	36.38	C
ATOM	701	C	SER A 617	-1.925	28.337	15.451	1.00	36.70	O
ATOM	702	O	SER A 617	-1.140	28.383	16.399	1.00	36.03	N
ATOM	703	N	ALA A 618	-1.953	27.331	14.577	1.00	37.72	C
ATOM	704	CA	ALA A 618	-1.035	26.182	14.640	1.00	38.97	C
ATOM	705	CB	ALA A 618	0.413	26.667	14.784	1.00	34.92	C
ATOM	706	C	ALA A 618	-1.374	25.205	15.766	1.00	40.28	O
ATOM	707	O	ALA A 618	-0.522	24.427	16.208	1.00	40.76	N
ATOM	708	N	ASN A 619	-2.625	25.241	16.216	1.00	40.30	C
ATOM	709	CA	ASN A 619	-3.083	24.371	17.291	1.00	41.16	C
ATOM	710	CB	ASN A 619	-4.241	25.038	18.042	1.00	39.96	C
ATOM	711	CG	ASN A 619	-3.772	26.123	18.985	1.00	41.03	O
ATOM	712	OD1	ASN A 619	-2.955	25.869	19.867	1.00	42.68	N
ATOM	713	ND2	ASN A 619	-4.286	27.338	18.811	1.00	38.42	C
ATOM	714	C	ASN A 619	-3.526	22.981	16.820	1.00	41.91	O
ATOM	715	O	ASN A 619	-2.945	21.957	17.208	1.00	42.47	N
ATOM	716	N	LEU A 620	-4.557	22.958	15.983	1.00	39.93	C
ATOM	717	CA	LEU A 620	-5.121	21.713	15.479	1.00	37.81	C
ATOM	718	CB	LEU A 620	-6.649	21.797	15.557	1.00	37.01	C
ATOM	719	CG	LEU A 620	-7.224	22.411	16.839	1.00	35.93	C
ATOM	720	CD1	LEU A 620	-8.301	23.406	16.460	1.00	33.11	C
ATOM	721	CD2	LEU A 620	-7.760	21.324	17.772	1.00	34.08	C
ATOM	722	C	LEU A 620	-4.703	21.439	14.035	1.00	36.13	C

ATOM	723	O	LEU A 620	-4.360	22.358	13.286	1.00	36.62	O
ATOM	724	N	LEU A 621	-4.727	20.171	13.644	1.00	32.72	N
ATOM	725	CA	LEU A 621	-4.391	19.833	12.274	1.00	28.31	C
ATOM	726	CB	LEU A 621	-3.902	18.386	12.164	1.00	26.41	C
ATOM	727	CG	LEU A 621	-2.447	18.262	11.699	1.00	25.72	C
ATOM	728	CD1	LEU A 621	-2.120	16.819	11.334	1.00	23.94	C
ATOM	729	CD2	LEU A 621	-2.229	19.159	10.507	1.00	25.40	C
ATOM	730	C	LEU A 621	-5.652	20.026	11.447	1.00	26.57	C
ATOM	731	O	LEU A 621	-6.627	19.296	11.600	1.00	25.08	O
ATOM	732	N	CYS A 622	-5.628	21.019	10.566	1.00	26.37	N
ATOM	733	CA	CYS A 622	-6.782	21.314	9.732	1.00	25.81	C
ATOM	734	CB	CYS A 622	-7.002	22.829	9.687	1.00	26.54	C
ATOM	735	SG	CYS A 622	-6.984	23.647	11.311	1.00	28.78	S
ATOM	736	C	CYS A 622	-6.658	20.756	8.309	1.00	24.71	C
ATOM	737	O	CYS A 622	-6.253	21.456	7.378	1.00	25.09	O
ATOM	738	N	PHE A 623	-7.008	19.489	8.137	1.00	24.71	N
ATOM	739	CA	PHE A 623	-6.945	18.878	6.808	1.00	23.70	C
ATOM	740	CB	PHE A 623	-7.243	17.386	6.881	1.00	18.33	C
ATOM	741	CG	PHE A 623	-6.162	16.582	7.526	1.00	16.85	C
ATOM	742	CD1	PHE A 623	-4.889	16.531	6.974	1.00	15.43	C
ATOM	743	CD2	PHE A 623	-6.427	15.831	8.667	1.00	17.87	C
ATOM	744	CE1	PHE A 623	-3.899	15.740	7.539	1.00	13.82	C
ATOM	745	CE2	PHE A 623	-5.440	15.037	9.241	1.00	18.17	C
ATOM	746	CZ	PHE A 623	-4.173	14.990	8.672	1.00	13.35	C
ATOM	747	C	PHE A 623	-7.967	19.537	5.893	1.00	23.13	C
ATOM	748	O	PHE A 623	-7.664	19.912	4.769	1.00	23.60	O
ATOM	749	N	ALA A 624	-9.186	19.669	6.392	1.00	25.10	N
ATOM	750	CA	ALA A 624	-10.265	20.275	5.630	1.00	25.37	C
ATOM	751	CB	ALA A 624	-11.019	19.204	4.850	1.00	22.60	C
ATOM	752	C	ALA A 624	-11.189	20.958	6.627	1.00	26.94	C
ATOM	753	O	ALA A 624	-11.253	20.553	7.791	1.00	26.03	O
ATOM	754	N	PRO A 625	-11.920	21.997	6.180	1.00	27.90	N
ATOM	755	CD	PRO A 625	-12.009	22.463	4.779	1.00	27.57	C
ATOM	756	CA	PRO A 625	-12.847	22.741	7.040	1.00	28.39	C
ATOM	757	CB	PRO A 625	-13.661	23.562	6.036	1.00	29.05	C
ATOM	758	CG	PRO A 625	-12.664	23.822	4.925	1.00	26.57	C
ATOM	759	C	PRO A 625	-13.724	21.826	7.900	1.00	29.86	C
ATOM	760	O	PRO A 625	-14.072	22.163	9.036	1.00	30.15	O
ATOM	761	N	ASP A 626	-14.059	20.658	7.363	1.00	30.80	N
ATOM	762	CA	ASP A 626	-14.906	19.704	8.079	1.00	31.85	C
ATOM	763	CB	ASP A 626	-16.034	19.232	7.160	1.00	32.39	C
ATOM	764	CG	ASP A 626	-15.519	18.523	5.938	1.00	34.23	C
ATOM	765	OD1	ASP A 626	-14.481	18.968	5.402	1.00	35.11	O
ATOM	766	OD2	ASP A 626	-16.147	17.529	5.510	1.00	36.31	O
ATOM	767	C	ASP A 626	-14.160	18.491	8.637	1.00	31.65	C
ATOM	768	O	ASP A 626	-14.784	17.490	8.998	1.00	31.79	O
ATOM	769	N	LEU A 627	-12.835	18.577	8.705	1.00	30.72	N
ATOM	770	CA	LEU A 627	-12.023	17.485	9.231	1.00	30.39	C
ATOM	771	CB	LEU A 627	-11.627	16.518	8.112	1.00	31.94	C
ATOM	772	CG	LEU A 627	-10.730	15.346	8.526	1.00	32.23	C
ATOM	773	CD1	LEU A 627	-11.443	14.478	9.540	1.00	32.57	C
ATOM	774	CD2	LEU A 627	-10.367	14.529	7.316	1.00	33.61	C
ATOM	775	C	LEU A 627	-10.776	18.051	9.904	1.00	30.91	C
ATOM	776	O	LEU A 627	-9.731	18.242	9.276	1.00	31.58	O
ATOM	777	N	ILE A 628	-10.915	18.315	11.197	1.00	30.42	N
ATOM	778	CA	ILE A 628	-9.861	18.872	12.019	1.00	29.12	C
ATOM	779	CB	ILE A 628	-10.332	20.201	12.619	1.00	29.30	C
ATOM	780	CG2	ILE A 628	-9.256	20.774	13.523	1.00	28.96	C
ATOM	781	CG1	ILE A 628	-10.691	21.165	11.481	1.00	29.83	C
ATOM	782	CD1	ILE A 628	-11.173	22.534	11.943	1.00	29.22	C
ATOM	783	C	ILE A 628	-9.500	17.884	13.132	1.00	28.55	C
ATOM	784	O	ILE A 628	-10.372	17.326	13.793	1.00	26.89	O
ATOM	785	N	ILE A 629	-8.206	17.671	13.332	1.00	28.07	N
ATOM	786	CA	ILE A 629	-7.738	16.735	14.342	1.00	28.14	C
ATOM	787	CB	ILE A 629	-6.417	16.059	13.894	1.00	23.41	C
ATOM	788	CG2	ILE A 629	-6.097	14.872	14.800	1.00	20.89	C

ATOM	789	CG1	ILE	A	629	-6.542	15.586	12.438	1.00	21.39	C
ATOM	790	CD1	ILE	A	629	-7.626	14.556	12.187	1.00	14.88	C
ATOM	791	C	ILE	A	629	-7.532	17.417	15.690	1.00	31.04	C
ATOM	792	O	ILE	A	629	-6.438	17.877	16.011	1.00	31.58	O
ATOM	793	N	ASN	A	630	-8.601	17.484	16.473	1.00	35.43	N
ATOM	794	CA	ASN	A	630	-8.546	18.094	17.795	1.00	40.50	C
ATOM	795	CB	ASN	A	630	-9.959	18.296	18.339	1.00	38.06	C
ATOM	796	CG	ASN	A	630	-10.785	17.039	18.260	1.00	38.08	C
ATOM	797	OD1	ASN	A	630	-11.849	17.018	17.639	1.00	40.80	O
ATOM	798	ND2	ASN	A	630	-10.300	15.976	18.881	1.00	35.09	N
ATOM	799	C	ASN	A	630	-7.751	17.207	18.750	1.00	43.32	C
ATOM	800	O	ASN	A	630	-7.347	16.096	18.395	1.00	42.91	O
ATOM	801	N	GLU	A	631	-7.548	17.706	19.965	1.00	47.18	N
ATOM	802	CA	GLU	A	631	-6.793	16.990	20.988	1.00	51.44	C
ATOM	803	CB	GLU	A	631	-6.699	17.832	22.266	1.00	54.29	C
ATOM	804	CG	GLU	A	631	-6.226	19.263	22.058	1.00	59.06	C
ATOM	805	CD	GLU	A	631	-7.322	20.281	22.336	1.00	61.38	C
ATOM	806	OE1	GLU	A	631	-8.355	20.250	21.624	1.00	61.72	O
ATOM	807	OE2	GLU	A	631	-7.149	21.105	23.267	1.00	62.30	O
ATOM	808	C	GLU	A	631	-7.372	15.622	21.342	1.00	52.40	C
ATOM	809	O	GLU	A	631	-6.630	14.729	21.751	1.00	53.22	O
ATOM	810	N	GLN	A	632	-8.685	15.451	21.195	1.00	53.21	N
ATOM	811	CA	GLN	A	632	-9.310	14.171	21.529	1.00	53.88	C
ATOM	812	CB	GLN	A	632	-10.754	14.378	21.999	1.00	55.39	C
ATOM	813	CG	GLN	A	632	-11.801	14.240	20.899	1.00	57.92	C
ATOM	814	CD	GLN	A	632	-13.221	14.366	21.425	1.00	60.19	C
ATOM	815	OE1	GLN	A	632	-13.605	13.685	22.380	1.00	60.31	O
ATOM	816	NE2	GLN	A	632	-14.013	15.234	20.796	1.00	60.27	N
ATOM	817	C	GLN	A	632	-9.305	13.201	20.354	1.00	53.11	C
ATOM	818	O	GLN	A	632	-9.185	11.988	20.535	1.00	53.30	O
ATOM	819	N	ARG	A	633	-9.444	13.741	19.150	1.00	51.68	N
ATOM	820	CA	ARG	A	633	-9.464	12.917	17.954	1.00	50.42	C
ATOM	821	CB	ARG	A	633	-10.052	13.700	16.780	1.00	49.64	C
ATOM	822	CG	ARG	A	633	-10.689	12.826	15.722	1.00	47.25	C
ATOM	823	CD	ARG	A	633	-10.664	13.514	14.376	1.00	45.91	C
ATOM	824	NE	ARG	A	633	-11.347	14.805	14.379	1.00	42.55	N
ATOM	825	CZ	ARG	A	633	-12.635	14.979	14.094	1.00	39.26	C
ATOM	826	NH1	ARG	A	633	-13.400	13.947	13.785	1.00	34.48	N
ATOM	827	NH2	ARG	A	633	-13.151	16.197	14.087	1.00	38.89	N
ATOM	828	C	ARG	A	633	-8.048	12.473	17.619	1.00	49.42	C
ATOM	829	O	ARG	A	633	-7.852	11.524	16.864	1.00	48.98	O
ATOM	830	N	MET	A	634	-7.063	13.160	18.188	1.00	48.32	N
ATOM	831	CA	MET	A	634	-5.678	12.816	17.935	1.00	48.72	C
ATOM	832	CB	MET	A	634	-4.802	14.064	17.966	1.00	49.49	C
ATOM	833	CG	MET	A	634	-3.509	13.872	17.211	1.00	49.15	C
ATOM	834	SD	MET	A	634	-2.588	15.371	17.083	1.00	51.35	S
ATOM	835	CE	MET	A	634	-3.431	16.197	15.727	1.00	51.40	C
ATOM	836	C	MET	A	634	-5.174	11.799	18.949	1.00	49.43	C
ATOM	837	O	MET	A	634	-3.972	11.534	19.045	1.00	49.13	O
ATOM	838	N	THR	A	635	-6.109	11.240	19.712	1.00	49.97	N
ATOM	839	CA	THR	A	635	-5.789	10.225	20.708	1.00	48.31	C
ATOM	840	CB	THR	A	635	-6.635	10.381	21.989	1.00	49.06	C
ATOM	841	OG1	THR	A	635	-7.985	9.966	21.736	1.00	49.20	O
ATOM	842	CG2	THR	A	635	-6.634	11.823	22.436	1.00	48.63	C
ATOM	843	C	THR	A	635	-6.107	8.879	20.079	1.00	46.80	C
ATOM	844	O	THR	A	635	-5.814	7.836	20.656	1.00	47.01	O
ATOM	845	N	LEU	A	636	-6.722	8.917	18.897	1.00	45.19	N
ATOM	846	CA	LEU	A	636	-7.061	7.703	18.161	1.00	44.54	C
ATOM	847	CB	LEU	A	636	-7.899	8.031	16.920	1.00	45.26	C
ATOM	848	CG	LEU	A	636	-9.396	8.298	17.073	1.00	46.68	C
ATOM	849	CD1	LEU	A	636	-9.640	9.415	18.072	1.00	48.83	C
ATOM	850	CD2	LEU	A	636	-9.972	8.670	15.715	1.00	47.31	C
ATOM	851	C	LEU	A	636	-5.774	7.008	17.723	1.00	42.83	C
ATOM	852	O	LEU	A	636	-4.752	7.654	17.502	1.00	41.79	O
ATOM	853	N	PRO	A	637	-5.812	5.674	17.600	1.00	42.87	N
ATOM	854	CD	PRO	A	637	-6.970	4.805	17.881	1.00	42.81	C

ATOM	855	CA	PRO	A	637	-4.655	4.873	17.188	1.00	42.64	C
ATOM	856	CB	PRO	A	637	-5.264	3.495	16.949	1.00	42.55	C
ATOM	857	CG	PRO	A	637	-6.325	3.436	18.000	1.00	42.89	C
ATOM	858	C	PRO	A	637	-3.943	5.404	15.948	1.00	42.03	C
ATOM	859	O	PRO	A	637	-4.545	5.526	14.875	1.00	41.50	O
ATOM	860	N	ASP	A	638	-2.659	5.713	16.121	1.00	41.66	N
ATOM	861	CA	ASP	A	638	-1.787	6.212	15.061	1.00	41.69	C
ATOM	862	CB	ASP	A	638	-1.949	5.369	13.794	1.00	44.86	C
ATOM	863	CG	ASP	A	638	-1.250	4.025	13.897	1.00	47.64	C
ATOM	864	OD1	ASP	A	638	-0.016	4.013	14.126	1.00	49.89	O
ATOM	865	OD2	ASP	A	638	-1.932	2.985	13.748	1.00	47.98	O
ATOM	866	C	ASP	A	638	-1.947	7.679	14.707	1.00	40.66	C
ATOM	867	O	ASP	A	638	-1.089	8.247	14.025	1.00	41.62	O
ATOM	868	N	MET	A	639	-3.032	8.297	15.163	1.00	37.51	N
ATOM	869	CA	MET	A	639	-3.250	9.699	14.860	1.00	35.41	C
ATOM	870	CB	MET	A	639	-4.546	10.196	15.495	1.00	35.58	C
ATOM	871	CG	MET	A	639	-5.760	10.003	14.605	1.00	37.29	C
ATOM	872	SD	MET	A	639	-5.504	10.544	12.886	1.00	37.08	S
ATOM	873	CE	MET	A	639	-5.554	8.978	12.096	1.00	37.85	C
ATOM	874	C	MET	A	639	-2.087	10.580	15.292	1.00	33.96	C
ATOM	875	O	MET	A	639	-1.552	11.346	14.488	1.00	34.72	O
ATOM	876	N	TYR	A	640	-1.681	10.465	16.550	1.00	31.47	N
ATOM	877	CA	TYR	A	640	-0.580	11.276	17.052	1.00	29.77	C
ATOM	878	CB	TYR	A	640	-0.353	11.022	18.551	1.00	27.01	C
ATOM	879	CG	TYR	A	640	0.952	11.622	19.059	1.00	25.22	C
ATOM	880	CD1	TYR	A	640	1.006	12.929	19.558	1.00	23.71	C
ATOM	881	CE1	TYR	A	640	2.224	13.499	19.967	1.00	22.51	C
ATOM	882	CD2	TYR	A	640	2.149	10.904	18.982	1.00	23.26	C
ATOM	883	CE2	TYR	A	640	3.372	11.473	19.383	1.00	21.37	C
ATOM	884	CZ	TYR	A	640	3.399	12.767	19.875	1.00	21.41	C
ATOM	885	OH	TYR	A	640	4.597	13.328	20.283	1.00	22.84	O
ATOM	886	C	TYR	A	640	0.745	11.057	16.325	1.00	28.18	C
ATOM	887	O	TYR	A	640	1.426	12.010	15.953	1.00	26.85	O
ATOM	888	N	ASP	A	641	1.117	9.797	16.151	1.00	28.71	N
ATOM	889	CA	ASP	A	641	2.380	9.453	15.517	1.00	28.19	C
ATOM	890	CB	ASP	A	641	2.471	7.947	15.339	1.00	28.67	C
ATOM	891	CG	ASP	A	641	3.813	7.512	14.820	1.00	29.28	C
ATOM	892	OD1	ASP	A	641	3.844	6.692	13.878	1.00	32.46	O
ATOM	893	OD2	ASP	A	641	4.838	7.985	15.353	1.00	30.37	O
ATOM	894	C	ASP	A	641	2.625	10.126	14.175	1.00	29.44	C
ATOM	895	O	ASP	A	641	3.686	10.707	13.951	1.00	30.37	O
ATOM	896	N	GLN	A	642	1.655	10.043	13.273	1.00	29.03	N
ATOM	897	CA	GLN	A	642	1.839	10.657	11.970	1.00	29.83	C
ATOM	898	CB	GLN	A	642	1.042	9.900	10.892	1.00	29.78	C
ATOM	899	CG	GLN	A	642	-0.397	9.609	11.246	1.00	32.54	C
ATOM	900	CD	GLN	A	642	-1.008	8.512	10.383	1.00	31.80	C
ATOM	901	OE1	GLN	A	642	-2.149	8.103	10.601	1.00	32.82	O
ATOM	902	NE2	GLN	A	642	-0.255	8.035	9.401	1.00	29.50	N
ATOM	903	C	GLN	A	642	1.495	12.135	11.958	1.00	29.04	C
ATOM	904	O	GLN	A	642	2.102	12.903	11.202	1.00	28.81	O
ATOM	905	N	CYS	A	643	0.551	12.536	12.809	1.00	26.79	N
ATOM	906	CA	CYS	A	643	0.143	13.934	12.882	1.00	25.81	C
ATOM	907	CB	CYS	A	643	-1.111	14.087	13.742	1.00	26.43	C
ATOM	908	SG	CYS	A	643	-2.642	13.720	12.873	1.00	28.94	S
ATOM	909	C	CYS	A	643	1.203	14.890	13.404	1.00	25.12	C
ATOM	910	O	CYS	A	643	1.236	16.046	12.996	1.00	27.03	O
ATOM	911	N	LYS	A	644	2.059	14.422	14.304	1.00	23.52	N
ATOM	912	CA	LYS	A	644	3.100	15.274	14.886	1.00	24.89	C
ATOM	913	CB	LYS	A	644	3.893	14.502	15.959	1.00	25.80	C
ATOM	914	CG	LYS	A	644	4.718	13.327	15.415	1.00	24.01	C
ATOM	915	CD	LYS	A	644	5.496	12.621	16.497	1.00	20.96	C
ATOM	916	CE	LYS	A	644	6.247	11.448	15.906	1.00	23.30	C
ATOM	917	NZ	LYS	A	644	7.056	10.715	16.919	1.00	21.99	N
ATOM	918	C	LYS	A	644	4.070	15.820	13.845	1.00	24.66	C
ATOM	919	O	LYS	A	644	4.763	16.808	14.092	1.00	24.41	O
ATOM	920	N	HIS	A	645	4.124	15.160	12.690	1.00	25.17	N

ATOM	921	CA	HIS	A	645	5.011	15.559	11.605	1.00	23.72	C
ATOM	922	CB	HIS	A	645	5.247	14.369	10.665	1.00	24.16	C
ATOM	923	CG	HIS	A	645	5.923	13.202	11.322	1.00	25.02	C
ATOM	924	CD2	HIS	A	645	5.504	11.932	11.543	1.00	25.31	C
ATOM	925	ND1	HIS	A	645	7.191	13.283	11.858	1.00	26.18	N
ATOM	926	CE1	HIS	A	645	7.522	12.115	12.383	1.00	24.70	C
ATOM	927	NE2	HIS	A	645	6.516	11.278	12.206	1.00	22.90	N
ATOM	928	C	HIS	A	645	4.427	16.750	10.838	1.00	23.69	C
ATOM	929	O	HIS	A	645	5.160	17.643	10.401	1.00	23.05	O
ATOM	930	N	MET	A	646	3.106	16.753	10.677	1.00	23.32	N
ATOM	931	CA	MET	A	646	2.406	17.831	9.985	1.00	23.24	C
ATOM	932	CB	MET	A	646	1.001	17.372	9.566	1.00	23.98	C
ATOM	933	CG	MET	A	646	0.898	16.732	8.179	1.00	28.41	C
ATOM	934	SD	MET	A	646	0.483	14.969	8.154	1.00	27.09	S
ATOM	935	CE	MET	A	646	-1.059	14.932	8.869	1.00	31.59	C
ATOM	936	C	MET	A	646	2.276	19.035	10.917	1.00	22.15	C
ATOM	937	O	MET	A	646	2.276	20.185	10.484	1.00	23.45	O
ATOM	938	N	LEU	A	647	2.146	18.754	12.206	1.00	21.18	N
ATOM	939	CA	LEU	A	647	2.003	19.793	13.207	1.00	20.07	C
ATOM	940	CB	LEU	A	647	1.605	19.164	14.549	1.00	18.03	C
ATOM	941	CG	LEU	A	647	0.198	19.449	15.109	1.00	15.70	C
ATOM	942	CD1	LEU	A	647	-0.655	20.155	14.089	1.00	11.85	C
ATOM	943	CD2	LEU	A	647	-0.449	18.152	15.561	1.00	14.31	C
ATOM	944	C	LEU	A	647	3.317	20.559	13.323	1.00	21.04	C
ATOM	945	O	LEU	A	647	3.344	21.708	13.755	1.00	21.54	O
ATOM	946	N	TYR	A	648	4.409	19.919	12.918	1.00	22.12	N
ATOM	947	CA	TYR	A	648	5.716	20.553	12.953	1.00	22.89	C
ATOM	948	CB	TYR	A	648	6.801	19.553	12.579	1.00	25.18	C
ATOM	949	CG	TYR	A	648	8.142	20.210	12.380	1.00	27.21	C
ATOM	950	CD1	TYR	A	648	8.845	20.746	13.461	1.00	28.35	C
ATOM	951	CE1	TYR	A	648	10.072	21.388	13.272	1.00	30.85	C
ATOM	952	CD2	TYR	A	648	8.692	20.330	11.104	1.00	28.25	C
ATOM	953	CE2	TYR	A	648	9.913	20.969	10.900	1.00	31.81	C
ATOM	954	CZ	TYR	A	648	10.599	21.496	11.985	1.00	32.69	C
ATOM	955	OH	TYR	A	648	11.805	22.132	11.770	1.00	36.37	O
ATOM	956	C	TYR	A	648	5.753	21.722	11.965	1.00	23.32	C
ATOM	957	O	TYR	A	648	6.202	22.821	12.307	1.00	22.94	O
ATOM	958	N	VAL	A	649	5.285	21.464	10.740	1.00	21.39	N
ATOM	959	CA	VAL	A	649	5.245	22.470	9.677	1.00	20.14	C
ATOM	960	CB	VAL	A	649	4.615	21.896	8.386	1.00	18.93	C
ATOM	961	CG1	VAL	A	649	4.551	22.979	7.293	1.00	17.59	C
ATOM	962	CG2	VAL	A	649	5.420	20.700	7.914	1.00	19.84	C
ATOM	963	C	VAL	A	649	4.424	23.676	10.112	1.00	19.80	C
ATOM	964	O	VAL	A	649	4.860	24.810	9.997	1.00	17.72	O
ATOM	965	N	SER	A	650	3.222	23.407	10.597	1.00	22.59	N
ATOM	966	CA	SER	A	650	2.311	24.446	11.068	1.00	25.99	C
ATOM	967	CB	SER	A	650	1.011	23.805	11.546	1.00	25.58	C
ATOM	968	OG	SER	A	650	0.158	24.787	12.092	1.00	29.64	O
ATOM	969	C	SER	A	650	2.922	25.246	12.221	1.00	26.73	C
ATOM	970	O	SER	A	650	2.744	26.460	12.326	1.00	27.60	O
ATOM	971	N	SER	A	651	3.645	24.546	13.084	1.00	25.89	N
ATOM	972	CA	SER	A	651	4.280	25.162	14.233	1.00	24.96	C
ATOM	973	CB	SER	A	651	4.864	24.067	15.123	1.00	25.41	C
ATOM	974	OG	SER	A	651	5.076	24.550	16.425	1.00	29.08	O
ATOM	975	C	SER	A	651	5.378	26.145	13.803	1.00	24.90	C
ATOM	976	O	SER	A	651	5.460	27.260	14.328	1.00	22.26	O
ATOM	977	N	GLU	A	652	6.219	25.726	12.853	1.00	24.07	N
ATOM	978	CA	GLU	A	652	7.299	26.571	12.349	1.00	22.81	C
ATOM	979	CB	GLU	A	652	8.204	25.776	11.418	1.00	23.24	C
ATOM	980	CG	GLU	A	652	9.198	24.881	12.138	1.00	25.38	C
ATOM	981	CD	GLU	A	652	10.067	25.661	13.098	1.00	27.50	C
ATOM	982	OE1	GLU	A	652	9.634	25.905	14.251	1.00	26.18	O
ATOM	983	OE2	GLU	A	652	11.180	26.054	12.686	1.00	28.48	O
ATOM	984	C	GLU	A	652	6.770	27.806	11.625	1.00	24.78	C
ATOM	985	O	GLU	A	652	7.316	28.902	11.775	1.00	24.25	O
ATOM	986	N	LEU	A	653	5.714	27.632	10.835	1.00	24.91	N

ATOM	987	CA	LEU	A	653	5.111	28.752	10.122	1.00	26.26	C
ATOM	988	CB	LEU	A	653	3.923	28.278	9.277	1.00	26.67	C
ATOM	989	CG	LEU	A	653	4.109	27.866	7.810	1.00	26.12	C
ATOM	990	CD1	LEU	A	653	5.290	26.945	7.647	1.00	27.97	C
ATOM	991	CD2	LEU	A	653	2.840	27.176	7.330	1.00	25.50	C
ATOM	992	C	LEU	A	653	4.629	29.764	11.157	1.00	27.54	C
ATOM	993	O	LEU	A	653	4.724	30.972	10.946	1.00	29.31	O
ATOM	994	N	HIS	A	654	4.116	29.250	12.274	1.00	27.97	N
ATOM	995	CA	HIS	A	654	3.612	30.065	13.381	1.00	28.01	C
ATOM	996	CB	HIS	A	654	2.914	29.171	14.412	1.00	28.47	C
ATOM	997	CG	HIS	A	654	2.419	29.912	15.611	1.00	29.23	C
ATOM	998	CD2	HIS	A	654	2.849	29.919	16.894	1.00	31.02	C
ATOM	999	ND1	HIS	A	654	1.375	30.811	15.553	1.00	31.41	N
ATOM	1000	CE1	HIS	A	654	1.184	31.341	16.748	1.00	31.38	C
ATOM	1001	NE2	HIS	A	654	2.066	30.816	17.580	1.00	31.53	N
ATOM	1002	C	HIS	A	654	4.741	30.821	14.079	1.00	28.29	C
ATOM	1003	O	HIS	A	654	4.639	32.016	14.349	1.00	26.43	O
ATOM	1004	N	ARG	A	655	5.805	30.089	14.389	1.00	29.23	N
ATOM	1005	CA	ARG	A	655	6.973	30.636	15.056	1.00	30.11	C
ATOM	1006	CB	ARG	A	655	7.976	29.506	15.331	1.00	29.80	C
ATOM	1007	CG	ARG	A	655	9.261	29.948	16.015	1.00	30.65	C
ATOM	1008	CD	ARG	A	655	10.210	28.784	16.209	1.00	32.47	C
ATOM	1009	NE	ARG	A	655	10.829	28.332	14.963	1.00	35.16	N
ATOM	1010	CZ	ARG	A	655	11.812	28.976	14.334	1.00	36.76	C
ATOM	1011	NH1	ARG	A	655	12.291	30.112	14.829	1.00	37.45	N
ATOM	1012	NH2	ARG	A	655	12.337	28.472	13.222	1.00	35.49	N
ATOM	1013	C	ARG	A	655	7.612	31.717	14.180	1.00	31.54	C
ATOM	1014	O	ARG	A	655	7.825	32.847	14.622	1.00	33.82	O
ATOM	1015	N	LEU	A	656	7.912	31.356	12.937	1.00	32.33	N
ATOM	1016	CA	LEU	A	656	8.522	32.263	11.970	1.00	31.24	C
ATOM	1017	CB	LEU	A	656	9.011	31.457	10.755	1.00	29.19	C
ATOM	1018	CG	LEU	A	656	10.502	31.120	10.568	1.00	27.84	C
ATOM	1019	CD1	LEU	A	656	11.277	31.188	11.878	1.00	26.94	C
ATOM	1020	CD2	LEU	A	656	10.604	29.741	9.935	1.00	24.56	C
ATOM	1021	C	LEU	A	656	7.544	33.357	11.521	1.00	31.13	C
ATOM	1022	O	LEU	A	656	7.942	34.318	10.870	1.00	30.73	O
ATOM	1023	N	GLN	A	657	6.269	33.210	11.869	1.00	31.70	N
ATOM	1024	CA	GLN	A	657	5.266	34.201	11.491	1.00	33.08	C
ATOM	1025	CB	GLN	A	657	5.488	35.491	12.281	1.00	34.91	C
ATOM	1026	CG	GLN	A	657	4.979	35.436	13.708	1.00	35.94	C
ATOM	1027	CD	GLN	A	657	3.462	35.525	13.776	1.00	37.86	C
ATOM	1028	OE1	GLN	A	657	2.872	36.540	13.388	1.00	40.15	O
ATOM	1029	NE2	GLN	A	657	2.821	34.464	14.264	1.00	36.73	N
ATOM	1030	C	GLN	A	657	5.331	34.498	10.000	1.00	33.66	C
ATOM	1031	O	GLN	A	657	5.362	35.656	9.584	1.00	35.07	O
ATOM	1032	N	VAL	A	658	5.345	33.441	9.198	1.00	33.40	N
ATOM	1033	CA	VAL	A	658	5.425	33.579	7.751	1.00	31.86	C
ATOM	1034	CB	VAL	A	658	5.575	32.178	7.096	1.00	30.76	C
ATOM	1035	CG1	VAL	A	658	5.582	32.290	5.580	1.00	30.06	C
ATOM	1036	CG2	VAL	A	658	6.858	31.517	7.585	1.00	28.18	C
ATOM	1037	C	VAL	A	658	4.205	34.312	7.179	1.00	32.39	C
ATOM	1038	O	VAL	A	658	3.063	34.044	7.569	1.00	33.62	O
ATOM	1039	N	SER	A	659	4.454	35.250	6.268	1.00	30.95	N
ATOM	1040	CA	SER	A	659	3.380	36.008	5.638	1.00	29.99	C
ATOM	1041	CB	SER	A	659	3.882	37.373	5.160	1.00	29.29	C
ATOM	1042	OG	SER	A	659	4.689	37.247	3.996	1.00	28.31	O
ATOM	1043	C	SER	A	659	2.829	35.241	4.436	1.00	31.17	C
ATOM	1044	O	SER	A	659	3.484	34.356	3.882	1.00	31.99	O
ATOM	1045	N	TYR	A	660	1.627	35.601	4.018	1.00	30.55	N
ATOM	1046	CA	TYR	A	660	1.013	34.940	2.893	1.00	30.07	C
ATOM	1047	CB	TYR	A	660	-0.351	35.568	2.606	1.00	29.55	C
ATOM	1048	CG	TYR	A	660	-1.182	34.749	1.655	1.00	30.20	C
ATOM	1049	CD1	TYR	A	660	-1.374	33.383	1.869	1.00	28.71	C
ATOM	1050	CE1	TYR	A	660	-2.135	32.620	0.993	1.00	30.32	C
ATOM	1051	CD2	TYR	A	660	-1.778	35.335	0.538	1.00	31.60	C
ATOM	1052	CE2	TYR	A	660	-2.545	34.580	-0.345	1.00	32.04	C

ATOM	1053	CZ	TYR	A	660	-2.718	33.224	-0.112	1.00	31.02	C
ATOM	1054	OH	TYR	A	660	-3.477	32.476	-0.987	1.00	32.79	O
ATOM	1055	C	TYR	A	660	1.910	34.997	1.658	1.00	30.23	C
ATOM	1056	O	TYR	A	660	2.044	34.003	0.951	1.00	32.23	O
ATOM	1057	N	GLU	A	661	2.528	36.149	1.399	1.00	30.64	N
ATOM	1058	CA	GLU	A	661	3.417	36.298	0.243	1.00	30.01	C
ATOM	1059	CB	GLU	A	661	3.843	37.762	0.076	1.00	33.12	C
ATOM	1060	CG	GLU	A	661	3.002	38.513	-0.951	1.00	38.91	C
ATOM	1061	CD	GLU	A	661	3.534	39.908	-1.271	1.00	42.25	C
ATOM	1062	OE1	GLU	A	661	4.750	40.054	-1.560	1.00	44.50	O
ATOM	1063	OE2	GLU	A	661	2.725	40.860	-1.246	1.00	43.08	O
ATOM	1064	C	GLU	A	661	4.653	35.397	0.335	1.00	27.83	C
ATOM	1065	O	GLU	A	661	4.995	34.706	-0.625	1.00	26.41	O
ATOM	1066	N	GLU	A	662	5.327	35.406	1.483	1.00	26.22	N
ATOM	1067	CA	GLU	A	662	6.495	34.548	1.666	1.00	26.21	C
ATOM	1068	CB	GLU	A	662	7.054	34.685	3.087	1.00	27.13	C
ATOM	1069	CG	GLU	A	662	7.505	36.093	3.457	1.00	28.24	C
ATOM	1070	CD	GLU	A	662	7.866	36.230	4.929	1.00	27.93	C
ATOM	1071	OE1	GLU	A	662	7.131	35.688	5.783	1.00	27.43	O
ATOM	1072	OE2	GLU	A	662	8.877	36.893	5.234	1.00	28.04	O
ATOM	1073	C	GLU	A	662	6.052	33.102	1.443	1.00	25.09	C
ATOM	1074	O	GLU	A	662	6.745	32.321	0.795	1.00	24.70	O
ATOM	1075	N	TYR	A	663	4.879	32.772	1.985	1.00	23.13	N
ATOM	1076	CA	TYR	A	663	4.289	31.442	1.889	1.00	20.90	C
ATOM	1077	CB	TYR	A	663	2.921	31.435	2.559	1.00	21.82	C
ATOM	1078	CG	TYR	A	663	2.073	30.239	2.200	1.00	23.06	C
ATOM	1079	CD1	TYR	A	663	2.383	28.967	2.681	1.00	22.74	C
ATOM	1080	CE1	TYR	A	663	1.597	27.860	2.345	1.00	24.36	C
ATOM	1081	CD2	TYR	A	663	0.957	30.380	1.370	1.00	22.89	C
ATOM	1082	CE2	TYR	A	663	0.169	29.287	1.025	1.00	23.08	C
ATOM	1083	CZ	TYR	A	663	0.491	28.031	1.515	1.00	25.25	C
ATOM	1084	OH	TYR	A	663	-0.304	26.956	1.175	1.00	27.42	O
ATOM	1085	C	TYR	A	663	4.137	30.980	0.455	1.00	21.27	C
ATOM	1086	O	TYR	A	663	4.588	29.893	0.081	1.00	21.88	O
ATOM	1087	N	LEU	A	664	3.471	31.808	-0.339	1.00	20.62	N
ATOM	1088	CA	LEU	A	664	3.241	31.517	-1.739	1.00	19.11	C
ATOM	1089	CB	LEU	A	664	2.554	32.716	-2.396	1.00	19.47	C
ATOM	1090	CG	LEU	A	664	1.155	33.007	-1.857	1.00	20.24	C
ATOM	1091	CD1	LEU	A	664	0.595	34.269	-2.516	1.00	20.06	C
ATOM	1092	CD2	LEU	A	664	0.255	31.797	-2.121	1.00	19.53	C
ATOM	1093	C	LEU	A	664	4.552	31.205	-2.460	1.00	19.15	C
ATOM	1094	O	LEU	A	664	4.636	30.242	-3.237	1.00	17.94	O
ATOM	1095	N	CYS	A	665	5.567	32.025	-2.196	1.00	18.90	N
ATOM	1096	CA	CYS	A	665	6.882	31.858	-2.817	1.00	20.45	C
ATOM	1097	CB	CYS	A	665	7.771	33.086	-2.555	1.00	20.26	C
ATOM	1098	SG	CYS	A	665	7.156	34.628	-3.251	1.00	23.67	S
ATOM	1099	C	CYS	A	665	7.580	30.615	-2.296	1.00	18.73	C
ATOM	1100	O	CYS	A	665	8.315	29.964	-3.033	1.00	20.72	O
ATOM	1101	N	MET	A	666	7.353	30.292	-1.026	1.00	17.68	N
ATOM	1102	CA	MET	A	666	7.974	29.122	-0.418	1.00	18.39	C
ATOM	1103	CB	MET	A	666	7.800	29.152	1.108	1.00	17.75	C
ATOM	1104	CG	MET	A	666	8.714	30.158	1.813	1.00	17.57	C
ATOM	1105	SD	MET	A	666	8.402	30.362	3.585	1.00	20.65	S
ATOM	1106	CE	MET	A	666	9.480	29.066	4.293	1.00	16.96	C
ATOM	1107	C	MET	A	666	7.370	27.849	-0.985	1.00	20.00	C
ATOM	1108	O	MET	A	666	8.081	26.884	-1.257	1.00	20.98	O
ATOM	1109	N	LYS	A	667	6.055	27.846	-1.181	1.00	19.75	N
ATOM	1110	CA	LYS	A	667	5.414	26.657	-1.707	1.00	20.53	C
ATOM	1111	CB	LYS	A	667	3.893	26.811	-1.662	1.00	20.31	C
ATOM	1112	CG	LYS	A	667	3.169	25.517	-1.969	1.00	20.01	C
ATOM	1113	CD	LYS	A	667	1.812	25.443	-1.272	1.00	20.65	C
ATOM	1114	CE	LYS	A	667	0.907	26.618	-1.612	1.00	20.22	C
ATOM	1115	NZ	LYS	A	667	0.536	26.728	-3.056	1.00	19.41	N
ATOM	1116	C	LYS	A	667	5.903	26.340	-3.124	1.00	19.51	C
ATOM	1117	O	LYS	A	667	6.241	25.194	-3.430	1.00	19.25	O
ATOM	1118	N	THR	A	668	5.956	27.355	-3.981	1.00	18.62	N

ATOM	1119	CA	THR	A	668	6.436	27.155	-5.341	1.00	18.09	C
ATOM	1120	CB	THR	A	668	6.503	28.474	-6.145	1.00	18.36	C
ATOM	1121	OG1	THR	A	668	5.250	29.165	-6.068	1.00	20.06	O
ATOM	1122	CG2	THR	A	668	6.806	28.168	-7.605	1.00	16.41	C
ATOM	1123	C	THR	A	668	7.845	26.557	-5.278	1.00	18.79	C
ATOM	1124	O	THR	A	668	8.154	25.623	-6.015	1.00	19.57	O
ATOM	1125	N	LEU	A	669	8.698	27.094	-4.407	1.00	17.40	N
ATOM	1126	CA	LEU	A	669	10.051	26.561	-4.265	1.00	17.47	C
ATOM	1127	CB	LEU	A	669	10.838	27.363	-3.227	1.00	17.26	C
ATOM	1128	CG	LEU	A	669	11.230	28.785	-3.660	1.00	17.73	C
ATOM	1129	CD1	LEU	A	669	11.915	29.534	-2.513	1.00	17.23	C
ATOM	1130	CD2	LEU	A	669	12.152	28.694	-4.862	1.00	16.78	C
ATOM	1131	C	LEU	A	669	10.047	25.077	-3.882	1.00	18.88	C
ATOM	1132	O	LEU	A	669	10.972	24.344	-4.231	1.00	20.45	O
ATOM	1133	N	LEU	A	670	9.015	24.628	-3.168	1.00	18.85	N
ATOM	1134	CA	LEU	A	670	8.922	23.218	-2.786	1.00	17.50	C
ATOM	1135	CB	LEU	A	670	7.823	23.008	-1.743	1.00	16.39	C
ATOM	1136	CG	LEU	A	670	8.127	23.554	-0.345	1.00	16.07	C
ATOM	1137	CD1	LEU	A	670	6.959	23.225	0.576	1.00	14.22	C
ATOM	1138	CD2	LEU	A	670	9.430	22.953	0.182	1.00	10.78	C
ATOM	1139	C	LEU	A	670	8.640	22.335	-3.992	1.00	16.98	C
ATOM	1140	O	LEU	A	670	8.924	21.139	-3.981	1.00	17.59	O
ATOM	1141	N	LEU	A	671	8.071	22.924	-5.033	1.00	18.06	N
ATOM	1142	CA	LEU	A	671	7.762	22.183	-6.257	1.00	18.65	C
ATOM	1143	CB	LEU	A	671	6.894	23.041	-7.183	1.00	19.05	C
ATOM	1144	CG	LEU	A	671	5.893	22.436	-8.175	1.00	20.75	C
ATOM	1145	CD1	LEU	A	671	5.792	23.368	-9.379	1.00	18.13	C
ATOM	1146	CD2	LEU	A	671	6.317	21.057	-8.615	1.00	22.35	C
ATOM	1147	C	LEU	A	671	9.088	21.905	-6.954	1.00	19.74	C
ATOM	1148	O	LEU	A	671	9.214	20.965	-7.740	1.00	18.68	O
ATOM	1149	N	LEU	A	672	10.076	22.739	-6.636	1.00	20.29	N
ATOM	1150	CA	LEU	A	672	11.403	22.668	-7.233	1.00	20.68	C
ATOM	1151	CB	LEU	A	672	11.754	24.038	-7.831	1.00	19.45	C
ATOM	1152	CG	LEU	A	672	10.575	24.758	-8.510	1.00	18.14	C
ATOM	1153	CD1	LEU	A	672	10.983	26.155	-8.956	1.00	19.69	C
ATOM	1154	CD2	LEU	A	672	10.100	23.939	-9.697	1.00	17.20	C
ATOM	1155	C	LEU	A	672	12.475	22.279	-6.230	1.00	20.29	C
ATOM	1156	O	LEU	A	672	13.613	22.698	-6.365	1.00	21.35	O
ATOM	1157	N	SER	A	673	12.124	21.479	-5.232	1.00	22.83	N
ATOM	1158	CA	SER	A	673	13.098	21.093	-4.215	1.00	25.61	C
ATOM	1159	CB	SER	A	673	12.414	21.023	-2.849	1.00	25.01	C
ATOM	1160	OG	SER	A	673	11.273	20.171	-2.870	1.00	25.80	O
ATOM	1161	C	SER	A	673	13.866	19.797	-4.489	1.00	28.68	C
ATOM	1162	O	SER	A	673	14.851	19.516	-3.814	1.00	29.61	O
ATOM	1163	N	SER	A	674	13.416	19.017	-5.473	1.00	32.04	N
ATOM	1164	CA	SER	A	674	14.069	17.760	-5.851	1.00	33.89	C
ATOM	1165	CB	SER	A	674	13.298	16.559	-5.300	1.00	33.29	C
ATOM	1166	OG	SER	A	674	13.627	16.313	-3.947	1.00	34.50	O
ATOM	1167	C	SER	A	674	14.218	17.593	-7.367	1.00	35.70	C
ATOM	1168	O	SER	A	674	13.335	17.963	-8.136	1.00	36.96	O
ATOM	1169	N	VAL	A	675	15.344	17.024	-7.783	1.00	37.67	N
ATOM	1170	CA	VAL	A	675	15.637	16.785	-9.191	1.00	38.73	C
ATOM	1171	CB	VAL	A	675	16.597	17.879	-9.741	1.00	38.56	C
ATOM	1172	CG1	VAL	A	675	17.100	17.508	-11.134	1.00	39.62	C
ATOM	1173	CG2	VAL	A	675	15.867	19.217	-9.801	1.00	37.67	C
ATOM	1174	C	VAL	A	675	16.286	15.406	-9.313	1.00	40.02	C
ATOM	1175	O	VAL	A	675	16.931	14.941	-8.371	1.00	39.57	O
ATOM	1176	N	PRO	A	676	16.094	14.717	-10.459	1.00	41.60	N
ATOM	1177	CD	PRO	A	676	15.187	15.035	-11.578	1.00	41.87	C
ATOM	1178	CA	PRO	A	676	16.695	13.389	-10.644	1.00	42.00	C
ATOM	1179	CB	PRO	A	676	16.177	12.959	-12.017	1.00	41.77	C
ATOM	1180	CG	PRO	A	676	14.882	13.665	-12.136	1.00	41.87	C
ATOM	1181	C	PRO	A	676	18.214	13.508	-10.625	1.00	42.91	C
ATOM	1182	O	PRO	A	676	18.754	14.555	-10.972	1.00	42.14	O
ATOM	1183	N	LYS	A	677	18.900	12.445	-10.217	1.00	46.47	N
ATOM	1184	CA	LYS	A	677	20.365	12.459	-10.172	1.00	49.54	C

ATOM	1185	CB	LYS	A	677	20.912	11.094	-9.736	1.00	50.75	C
ATOM	1186	CG	LYS	A	677	21.510	11.038	-8.334	1.00	52.00	C
ATOM	1187	CD	LYS	A	677	20.443	11.011	-7.256	1.00	53.60	C
ATOM	1188	CE	LYS	A	677	21.029	10.647	-5.894	1.00	52.72	C
ATOM	1189	NZ	LYS	A	677	21.914	11.716	-5.362	1.00	54.17	N
ATOM	1190	C	LYS	A	677	20.941	12.799	-11.545	1.00	50.54	C
ATOM	1191	O	LYS	A	677	21.863	13.610	-11.659	1.00	50.25	O
ATOM	1192	N	ASP	A	678	20.389	12.175	-12.585	1.00	52.11	N
ATOM	1193	CA	ASP	A	678	20.854	12.397	-13.954	1.00	54.21	C
ATOM	1194	CB	ASP	A	678	20.415	11.227	-14.848	1.00	56.12	C
ATOM	1195	CG	ASP	A	678	18.959	10.835	-14.634	1.00	59.10	C
ATOM	1196	OD1	ASP	A	678	18.053	11.617	-15.004	1.00	59.04	O
ATOM	1197	OD2	ASP	A	678	18.721	9.735	-14.087	1.00	61.96	O
ATOM	1198	C	ASP	A	678	20.406	13.731	-14.569	1.00	53.68	C
ATOM	1199	O	ASP	A	678	20.740	14.038	-15.718	1.00	54.41	O
ATOM	1200	N	GLY	A	679	19.656	14.520	-13.803	1.00	51.40	N
ATOM	1201	CA	GLY	A	679	19.192	15.802	-14.296	1.00	49.06	C
ATOM	1202	C	GLY	A	679	17.871	15.762	-15.050	1.00	48.05	C
ATOM	1203	O	GLY	A	679	17.336	14.694	-15.352	1.00	47.80	O
ATOM	1204	N	LEU	A	680	17.347	16.945	-15.356	1.00	46.40	N
ATOM	1205	CA	LEU	A	680	16.087	17.085	-16.070	1.00	45.15	C
ATOM	1206	CB	LEU	A	680	15.327	18.307	-15.548	1.00	44.21	C
ATOM	1207	CG	LEU	A	680	14.969	18.341	-14.058	1.00	42.73	C
ATOM	1208	CD1	LEU	A	680	14.546	19.743	-13.670	1.00	42.42	C
ATOM	1209	CD2	LEU	A	680	13.863	17.345	-13.767	1.00	39.89	C
ATOM	1210	C	LEU	A	680	16.344	17.259	-17.557	1.00	45.21	C
ATOM	1211	O	LEU	A	680	17.495	17.269	-18.000	1.00	45.81	O
ATOM	1212	N	LYS	A	681	15.269	17.390	-18.327	1.00	45.24	N
ATOM	1213	CA	LYS	A	681	15.398	17.589	-19.765	1.00	46.30	C
ATOM	1214	CB	LYS	A	681	14.024	17.562	-20.451	1.00	48.09	C
ATOM	1215	CG	LYS	A	681	13.602	16.210	-21.002	1.00	49.65	C
ATOM	1216	CD	LYS	A	681	13.266	15.222	-19.899	1.00	52.60	C
ATOM	1217	CE	LYS	A	681	12.731	13.922	-20.483	1.00	53.40	C
ATOM	1218	NZ	LYS	A	681	11.558	14.171	-21.370	1.00	53.89	N
ATOM	1219	C	LYS	A	681	16.059	18.945	-19.992	1.00	45.35	C
ATOM	1220	O	LYS	A	681	17.096	19.046	-20.650	1.00	46.12	O
ATOM	1221	N	SER	A	682	15.452	19.987	-19.440	1.00	44.06	N
ATOM	1222	CA	SER	A	682	15.993	21.329	-19.566	1.00	44.15	C
ATOM	1223	CB	SER	A	682	14.959	22.266	-20.200	1.00	46.02	C
ATOM	1224	OG	SER	A	682	13.738	22.262	-19.483	1.00	48.76	O
ATOM	1225	C	SER	A	682	16.413	21.848	-18.198	1.00	42.78	C
ATOM	1226	O	SER	A	682	15.763	22.722	-17.626	1.00	41.63	O
ATOM	1227	N	GLN	A	683	17.506	21.290	-17.683	1.00	42.98	N
ATOM	1228	CA	GLN	A	683	18.047	21.676	-16.384	1.00	44.09	C
ATOM	1229	CB	GLN	A	683	19.311	20.868	-16.068	1.00	44.53	C
ATOM	1230	CG	GLN	A	683	19.841	21.074	-14.653	1.00	46.82	C
ATOM	1231	CD	GLN	A	683	19.056	20.299	-13.593	1.00	49.02	C
ATOM	1232	OE1	GLN	A	683	19.036	20.677	-12.421	1.00	50.99	O
ATOM	1233	NE2	GLN	A	683	18.425	19.203	-14.000	1.00	50.06	N
ATOM	1234	C	GLN	A	683	18.393	23.159	-16.363	1.00	44.36	C
ATOM	1235	O	GLN	A	683	18.298	23.812	-15.327	1.00	44.59	O
ATOM	1236	N	GLU	A	684	18.792	23.682	-17.519	1.00	45.31	N
ATOM	1237	CA	GLU	A	684	19.175	25.083	-17.645	1.00	45.83	C
ATOM	1238	CB	GLU	A	684	19.847	25.333	-19.004	1.00	50.00	C
ATOM	1239	CG	GLU	A	684	21.116	24.496	-19.245	1.00	53.64	C
ATOM	1240	CD	GLU	A	684	20.818	23.036	-19.602	1.00	57.38	C
ATOM	1241	OE1	GLU	A	684	21.762	22.209	-19.571	1.00	59.95	O
ATOM	1242	OE2	GLU	A	684	19.648	22.718	-19.923	1.00	57.21	O
ATOM	1243	C	GLU	A	684	18.001	26.031	-17.464	1.00	43.87	C
ATOM	1244	O	GLU	A	684	18.155	27.116	-16.901	1.00	43.94	O
ATOM	1245	N	LEU	A	685	16.831	25.633	-17.951	1.00	41.57	N
ATOM	1246	CA	LEU	A	685	15.643	26.462	-17.798	1.00	39.24	C
ATOM	1247	CB	LEU	A	685	14.511	25.938	-18.678	1.00	39.22	C
ATOM	1248	CG	LEU	A	685	13.402	26.890	-19.154	1.00	38.34	C
ATOM	1249	CD1	LEU	A	685	12.294	26.052	-19.789	1.00	38.02	C
ATOM	1250	CD2	LEU	A	685	12.843	27.714	-18.006	1.00	36.92	C

ATOM	1251	C	LEU	A	685	15.234	26.358	-16.330	1.00	38.89	C
ATOM	1252	O	LEU	A	685	14.934	27.358	-15.678	1.00	38.67	O
ATOM	1253	N	PHE	A	686	15.235	25.131	-15.821	1.00	38.06	N
ATOM	1254	CA	PHE	A	686	14.878	24.861	-14.435	1.00	36.79	C
ATOM	1255	CB	PHE	A	686	15.182	23.399	-14.095	1.00	34.50	C
ATOM	1256	CG	PHE	A	686	14.911	23.045	-12.659	1.00	31.05	C
ATOM	1257	CD1	PHE	A	686	13.617	22.828	-12.217	1.00	28.43	C
ATOM	1258	CD2	PHE	A	686	15.952	22.983	-11.741	1.00	31.24	C
ATOM	1259	CE1	PHE	A	686	13.356	22.559	-10.883	1.00	29.05	C
ATOM	1260	CE2	PHE	A	686	15.706	22.715	-10.401	1.00	32.60	C
ATOM	1261	CZ	PHE	A	686	14.399	22.503	-9.970	1.00	32.35	C
ATOM	1262	C	PHE	A	686	15.618	25.781	-13.448	1.00	38.31	C
ATOM	1263	O	PHE	A	686	14.987	26.468	-12.637	1.00	37.53	O
ATOM	1264	N	ASP	A	687	16.950	25.788	-13.512	1.00	38.62	N
ATOM	1265	CA	ASP	A	687	17.751	26.621	-12.617	1.00	38.86	C
ATOM	1266	CB	ASP	A	687	19.238	26.582	-12.999	1.00	39.39	C
ATOM	1267	CG	ASP	A	687	19.834	25.179	-12.935	1.00	41.58	C
ATOM	1268	OD1	ASP	A	687	19.569	24.444	-11.952	1.00	42.64	O
ATOM	1269	OD2	ASP	A	687	20.586	24.821	-13.869	1.00	39.90	O
ATOM	1270	C	ASP	A	687	17.274	28.071	-12.642	1.00	39.11	C
ATOM	1271	O	ASP	A	687	17.254	28.740	-11.613	1.00	39.52	O
ATOM	1272	N	GLU	A	688	16.896	28.561	-13.816	1.00	38.90	N
ATOM	1273	CA	GLU	A	688	16.427	29.936	-13.920	1.00	40.57	C
ATOM	1274	CB	GLU	A	688	16.232	30.349	-15.382	1.00	43.83	C
ATOM	1275	CG	GLU	A	688	17.391	29.977	-16.285	1.00	51.85	C
ATOM	1276	CD	GLU	A	688	17.237	30.517	-17.702	1.00	56.49	C
ATOM	1277	OE1	GLU	A	688	17.963	30.027	-18.598	1.00	58.12	O
ATOM	1278	OE2	GLU	A	688	16.406	31.433	-17.917	1.00	58.33	O
ATOM	1279	C	GLU	A	688	15.113	30.094	-13.180	1.00	37.92	C
ATOM	1280	O	GLU	A	688	14.974	30.991	-12.359	1.00	38.28	O
ATOM	1281	N	ILE	A	689	14.155	29.220	-13.481	1.00	35.67	N
ATOM	1282	CA	ILE	A	689	12.840	29.251	-12.845	1.00	32.76	C
ATOM	1283	CB	ILE	A	689	11.963	28.035	-13.245	1.00	32.74	C
ATOM	1284	CG2	ILE	A	689	10.568	28.205	-12.663	1.00	32.12	C
ATOM	1285	CG1	ILE	A	689	11.888	27.897	-14.766	1.00	33.76	C
ATOM	1286	CD1	ILE	A	689	11.097	26.673	-15.241	1.00	31.81	C
ATOM	1287	C	ILE	A	689	12.972	29.215	-11.327	1.00	30.27	C
ATOM	1288	O	ILE	A	689	12.295	29.959	-10.616	1.00	29.85	O
ATOM	1289	N	ARG	A	690	13.838	28.339	-10.831	1.00	27.25	N
ATOM	1290	CA	ARG	A	690	14.020	28.217	-9.394	1.00	26.70	C
ATOM	1291	CB	ARG	A	690	14.901	27.013	-9.061	1.00	26.23	C
ATOM	1292	CG	ARG	A	690	14.970	26.699	-7.570	1.00	29.83	C
ATOM	1293	CD	ARG	A	690	15.202	25.214	-7.333	1.00	32.12	C
ATOM	1294	NE	ARG	A	690	15.257	24.868	-5.916	1.00	32.91	N
ATOM	1295	CZ	ARG	A	690	16.268	25.183	-5.113	1.00	35.77	C
ATOM	1296	NH1	ARG	A	690	17.307	25.852	-5.598	1.00	35.02	N
ATOM	1297	NH2	ARG	A	690	16.242	24.833	-3.828	1.00	35.15	N
ATOM	1298	C	ARG	A	690	14.624	29.481	-8.811	1.00	25.65	C
ATOM	1299	O	ARG	A	690	14.284	29.877	-7.697	1.00	25.19	O
ATOM	1300	N	MET	A	691	15.504	30.122	-9.575	1.00	25.28	N
ATOM	1301	CA	MET	A	691	16.157	31.346	-9.127	1.00	26.88	C
ATOM	1302	CB	MET	A	691	17.350	31.684	-10.034	1.00	27.69	C
ATOM	1303	CG	MET	A	691	18.200	32.878	-9.583	1.00	28.87	C
ATOM	1304	SD	MET	A	691	18.966	32.706	-7.929	1.00	33.69	S
ATOM	1305	CE	MET	A	691	20.087	31.350	-8.203	1.00	31.56	C
ATOM	1306	C	MET	A	691	15.199	32.531	-9.078	1.00	27.25	C
ATOM	1307	O	MET	A	691	15.249	33.325	-8.143	1.00	27.08	O
ATOM	1308	N	THR	A	692	14.311	32.655	-10.060	1.00	27.92	N
ATOM	1309	CA	THR	A	692	13.405	33.795	-10.034	1.00	29.53	C
ATOM	1310	CB	THR	A	692	12.590	33.944	-11.361	1.00	28.67	C
ATOM	1311	OG1	THR	A	692	11.290	33.365	-11.213	1.00	32.07	O
ATOM	1312	CG2	THR	A	692	13.319	33.282	-12.508	1.00	28.06	C
ATOM	1313	C	THR	A	692	12.464	33.728	-8.832	1.00	29.68	C
ATOM	1314	O	THR	A	692	12.056	34.770	-8.306	1.00	30.95	O
ATOM	1315	N	TYR	A	693	12.139	32.513	-8.385	1.00	29.07	N
ATOM	1316	CA	TYR	A	693	11.262	32.348	-7.230	1.00	28.24	C

ATOM	1317	CB	TYR	A	693	10.588	30.979	-7.248	1.00	27.45	C
ATOM	1318	CG	TYR	A	693	9.448	30.953	-8.226	1.00	27.19	C
ATOM	1319	CD1	TYR	A	693	8.343	31.790	-8.050	1.00	27.66	C
ATOM	1320	CE1	TYR	A	693	7.327	31.845	-9.004	1.00	28.20	C
ATOM	1321	CD2	TYR	A	693	9.506	30.161	-9.371	1.00	25.22	C
ATOM	1322	CE2	TYR	A	693	8.505	30.205	-10.325	1.00	24.86	C
ATOM	1323	CZ	TYR	A	693	7.418	31.050	-10.145	1.00	26.65	C
ATOM	1324	OH	TYR	A	693	6.444	31.123	-11.121	1.00	26.67	O
ATOM	1325	C	TYR	A	693	12.019	32.556	-5.933	1.00	27.30	C
ATOM	1326	O	TYR	A	693	11.431	32.899	-4.916	1.00	26.95	O
ATOM	1327	N	ILE	A	694	13.329	32.341	-5.976	1.00	25.29	N
ATOM	1328	CA	ILE	A	694	14.166	32.566	-4.810	1.00	22.49	C
ATOM	1329	CB	ILE	A	694	15.590	32.020	-5.043	1.00	22.05	C
ATOM	1330	CG2	ILE	A	694	16.555	32.558	-3.975	1.00	20.21	C
ATOM	1331	CG1	ILE	A	694	15.548	30.492	-5.057	1.00	20.54	C
ATOM	1332	CD1	ILE	A	694	16.820	29.831	-5.541	1.00	19.18	C
ATOM	1333	C	ILE	A	694	14.211	34.079	-4.615	1.00	22.37	C
ATOM	1334	O	ILE	A	694	14.083	34.575	-3.498	1.00	21.44	O
ATOM	1335	N	LYS	A	695	14.385	34.814	-5.711	1.00	22.80	N
ATOM	1336	CA	LYS	A	695	14.418	36.270	-5.639	1.00	25.33	C
ATOM	1337	CB	LYS	A	695	14.918	36.866	-6.961	1.00	25.07	C
ATOM	1338	CG	LYS	A	695	16.230	36.247	-7.420	1.00	30.28	C
ATOM	1339	CD	LYS	A	695	17.228	37.278	-7.965	1.00	32.15	C
ATOM	1340	CE	LYS	A	695	16.937	37.648	-9.407	1.00	30.01	C
ATOM	1341	NZ	LYS	A	695	16.956	36.441	-10.256	1.00	28.26	N
ATOM	1342	C	LYS	A	695	13.010	36.782	-5.319	1.00	25.73	C
ATOM	1343	O	LYS	A	695	12.844	37.826	-4.694	1.00	24.12	O
ATOM	1344	N	GLU	A	696	11.996	36.034	-5.739	1.00	27.02	N
ATOM	1345	CA	GLU	A	696	10.621	36.435	-5.468	1.00	30.00	C
ATOM	1346	CB	GLU	A	696	9.652	35.558	-6.266	1.00	31.62	C
ATOM	1347	CG	GLU	A	696	8.249	36.134	-6.443	1.00	35.63	C
ATOM	1348	CD	GLU	A	696	8.238	37.501	-7.113	1.00	37.94	C
ATOM	1349	OE1	GLU	A	696	8.967	37.685	-8.115	1.00	38.78	O
ATOM	1350	OE2	GLU	A	696	7.486	38.388	-6.640	1.00	37.89	O
ATOM	1351	C	GLU	A	696	10.388	36.299	-3.957	1.00	30.21	C
ATOM	1352	O	GLU	A	696	9.678	37.108	-3.353	1.00	31.90	O
ATOM	1353	N	LEU	A	697	10.998	35.282	-3.345	1.00	29.07	N
ATOM	1354	CA	LEU	A	697	10.882	35.086	-1.902	1.00	27.69	C
ATOM	1355	CB	LEU	A	697	11.573	33.786	-1.466	1.00	24.96	C
ATOM	1356	CG	LEU	A	697	11.774	33.592	0.047	1.00	25.29	C
ATOM	1357	CD1	LEU	A	697	10.430	33.618	0.760	1.00	24.14	C
ATOM	1358	CD2	LEU	A	697	12.495	32.281	0.321	1.00	24.08	C
ATOM	1359	C	LEU	A	697	11.561	36.287	-1.235	1.00	28.29	C
ATOM	1360	O	LEU	A	697	11.003	36.912	-0.331	1.00	28.81	O
ATOM	1361	N	GLY	A	698	12.767	36.604	-1.699	1.00	27.70	N
ATOM	1362	CA	GLY	A	698	13.499	37.738	-1.165	1.00	28.21	C
ATOM	1363	C	GLY	A	698	12.693	39.028	-1.213	1.00	28.68	C
ATOM	1364	O	GLY	A	698	12.801	39.870	-0.315	1.00	28.71	O
ATOM	1365	N	LYS	A	699	11.890	39.198	-2.260	1.00	28.92	N
ATOM	1366	CA	LYS	A	699	11.054	40.391	-2.372	1.00	30.57	C
ATOM	1367	CB	LYS	A	699	10.401	40.485	-3.753	1.00	31.39	C
ATOM	1368	CG	LYS	A	699	11.356	40.713	-4.907	1.00	32.68	C
ATOM	1369	CD	LYS	A	699	10.593	40.787	-6.224	1.00	35.34	C
ATOM	1370	CE	LYS	A	699	11.555	40.849	-7.402	1.00	38.47	C
ATOM	1371	NZ	LYS	A	699	10.872	41.099	-8.705	1.00	36.39	N
ATOM	1372	C	LYS	A	699	9.955	40.375	-1.309	1.00	30.15	C
ATOM	1373	O	LYS	A	699	9.525	41.428	-0.856	1.00	32.11	O
ATOM	1374	N	ALA	A	700	9.503	39.186	-0.916	1.00	29.32	N
ATOM	1375	CA	ALA	A	700	8.453	39.065	0.100	1.00	30.48	C
ATOM	1376	CB	ALA	A	700	7.800	37.681	0.027	1.00	30.02	C
ATOM	1377	C	ALA	A	700	9.018	39.311	1.497	1.00	31.46	C
ATOM	1378	O	ALA	A	700	8.330	39.845	2.374	1.00	31.19	O
ATOM	1379	N	ILE	A	701	10.273	38.917	1.698	1.00	32.63	N
ATOM	1380	CA	ILE	A	701	10.941	39.117	2.977	1.00	33.82	C
ATOM	1381	CB	ILE	A	701	12.260	38.325	3.063	1.00	32.82	C
ATOM	1382	CG2	ILE	A	701	12.987	38.673	4.370	1.00	31.37	C

ATOM	1383	CG1	ILE	A	701	11.975	36.827	2.951	1.00	29.56	C
ATOM	1384	CD1	ILE	A	701	13.201	35.960	3.037	1.00	28.16	C
ATOM	1385	C	ILE	A	701	11.274	40.595	3.142	1.00	36.47	C
ATOM	1386	O	ILE	A	701	11.193	41.149	4.240	1.00	36.90	O
ATOM	1387	N	VAL	A	702	11.662	41.229	2.042	1.00	39.58	N
ATOM	1388	CA	VAL	A	702	12.002	42.640	2.070	1.00	42.77	C
ATOM	1389	CB	VAL	A	702	12.752	43.057	0.791	1.00	42.44	C
ATOM	1390	CG1	VAL	A	702	12.914	44.569	0.741	1.00	41.22	C
ATOM	1391	CG2	VAL	A	702	14.112	42.389	0.767	1.00	42.49	C
ATOM	1392	C	VAL	A	702	10.733	43.460	2.221	1.00	45.14	C
ATOM	1393	O	VAL	A	702	10.705	44.432	2.978	1.00	46.12	O
ATOM	1394	N	LYS	A	703	9.684	43.062	1.506	1.00	47.91	N
ATOM	1395	CA	LYS	A	703	8.403	43.756	1.584	1.00	51.90	C
ATOM	1396	CB	LYS	A	703	7.341	43.029	0.750	1.00	51.46	C
ATOM	1397	CG	LYS	A	703	5.997	43.747	0.688	1.00	51.03	C
ATOM	1398	CD	LYS	A	703	5.135	43.208	-0.447	1.00	51.73	C
ATOM	1399	CE	LYS	A	703	3.858	44.012	-0.611	1.00	50.49	C
ATOM	1400	NZ	LYS	A	703	3.125	43.619	-1.845	1.00	51.56	N
ATOM	1401	C	LYS	A	703	7.977	43.798	3.048	1.00	55.10	C
ATOM	1402	O	LYS	A	703	7.328	44.742	3.490	1.00	55.48	O
ATOM	1403	N	ARG	A	704	8.352	42.762	3.792	1.00	59.04	N
ATOM	1404	CA	ARG	A	704	8.047	42.671	5.215	1.00	62.52	C
ATOM	1405	CB	ARG	A	704	8.384	41.262	5.712	1.00	61.41	C
ATOM	1406	CG	ARG	A	704	7.514	40.737	6.833	1.00	59.47	C
ATOM	1407	CD	ARG	A	704	7.402	39.226	6.714	1.00	59.10	C
ATOM	1408	NE	ARG	A	704	6.822	38.601	7.898	1.00	58.65	N
ATOM	1409	CZ	ARG	A	704	7.410	38.578	9.090	1.00	59.78	C
ATOM	1410	NH1	ARG	A	704	8.597	39.149	9.253	1.00	60.35	N
ATOM	1411	NH2	ARG	A	704	6.818	37.982	10.119	1.00	59.74	N
ATOM	1412	C	ARG	A	704	8.956	43.721	5.857	1.00	65.69	C
ATOM	1413	O	ARG	A	704	8.757	44.918	5.647	1.00	66.70	O
ATOM	1414	N	GLU	A	705	9.956	43.285	6.619	1.00	68.89	N
ATOM	1415	CA	GLU	A	705	10.898	44.218	7.240	1.00	71.53	C
ATOM	1416	CB	GLU	A	705	10.193	45.121	8.267	1.00	70.37	C
ATOM	1417	CG	GLU	A	705	9.634	46.411	7.672	1.00	68.88	C
ATOM	1418	CD	GLU	A	705	10.556	47.019	6.622	1.00	67.84	C
ATOM	1419	OE1	GLU	A	705	11.718	47.342	6.952	1.00	66.93	O
ATOM	1420	OE2	GLU	A	705	10.117	47.171	5.463	1.00	67.14	O
ATOM	1421	C	GLU	A	705	12.142	43.596	7.886	1.00	73.65	C
ATOM	1422	O	GLU	A	705	12.179	42.406	8.239	1.00	73.25	O
ATOM	1423	N	GLY	A	706	13.158	44.444	8.028	1.00	75.72	N
ATOM	1424	CA	GLY	A	706	14.427	44.056	8.613	1.00	77.54	C
ATOM	1425	C	GLY	A	706	15.432	45.157	8.325	1.00	78.76	C
ATOM	1426	O	GLY	A	706	15.403	45.767	7.249	1.00	77.81	O
ATOM	1427	N	ASN	A	707	16.313	45.426	9.285	1.00	80.16	N
ATOM	1428	CA	ASN	A	707	17.322	46.466	9.116	1.00	81.05	C
ATOM	1429	CB	ASN	A	707	17.788	46.987	10.485	1.00	81.76	C
ATOM	1430	CG	ASN	A	707	18.264	48.441	10.439	1.00	81.96	C
ATOM	1431	OD1	ASN	A	707	19.170	48.792	9.677	1.00	81.94	O
ATOM	1432	ND2	ASN	A	707	17.652	49.290	11.264	1.00	80.25	N
ATOM	1433	C	ASN	A	707	18.504	45.885	8.343	1.00	81.72	C
ATOM	1434	O	ASN	A	707	19.637	45.881	8.831	1.00	82.56	O
ATOM	1435	N	SER	A	708	18.219	45.381	7.141	1.00	81.77	N
ATOM	1436	CA	SER	A	708	19.228	44.788	6.260	1.00	80.86	C
ATOM	1437	CB	SER	A	708	20.302	45.832	5.914	1.00	81.99	C
ATOM	1438	OG	SER	A	708	21.266	45.310	5.012	1.00	82.02	O
ATOM	1439	C	SER	A	708	19.895	43.538	6.844	1.00	79.74	C
ATOM	1440	O	SER	A	708	20.396	42.690	6.101	1.00	79.98	O
ATOM	1441	N	SER	A	709	19.897	43.427	8.170	1.00	77.83	N
ATOM	1442	CA	SER	A	709	20.510	42.287	8.849	1.00	75.92	C
ATOM	1443	CB	SER	A	709	21.209	42.755	10.128	1.00	75.37	C
ATOM	1444	OG	SER	A	709	22.195	43.728	9.838	1.00	76.62	O
ATOM	1445	C	SER	A	709	19.496	41.199	9.198	1.00	73.87	C
ATOM	1446	O	SER	A	709	19.838	40.013	9.254	1.00	72.97	O
ATOM	1447	N	GLN	A	710	18.252	41.609	9.434	1.00	71.52	N
ATOM	1448	CA	GLN	A	710	17.206	40.662	9.787	1.00	68.86	C

ATOM	1449	CB	GLN	A	710	16.140	41.340	10.654	1.00	71.12	C
ATOM	1450	CG	GLN	A	710	15.270	40.349	11.431	1.00	73.78	C
ATOM	1451	CD	GLN	A	710	16.091	39.273	12.145	1.00	74.98	C
ATOM	1452	OE1	GLN	A	710	17.012	39.580	12.907	1.00	75.50	O
ATOM	1453	NE2	GLN	A	710	15.754	38.006	11.900	1.00	75.45	N
ATOM	1454	C	GLN	A	710	16.567	40.018	8.560	1.00	65.05	C
ATOM	1455	O	GLN	A	710	16.099	38.882	8.630	1.00	64.34	O
ATOM	1456	N	ASN	A	711	16.540	40.735	7.437	1.00	60.66	N
ATOM	1457	CA	ASN	A	711	15.978	40.151	6.228	1.00	55.86	C
ATOM	1458	CB	ASN	A	711	15.851	41.194	5.107	1.00	56.63	C
ATOM	1459	CG	ASN	A	711	16.898	42.283	5.186	1.00	57.48	C
ATOM	1460	OD1	ASN	A	711	18.094	42.010	5.221	1.00	58.78	O
ATOM	1461	ND2	ASN	A	711	16.449	43.533	5.198	1.00	58.96	N
ATOM	1462	C	ASN	A	711	16.845	38.962	5.786	1.00	51.87	C
ATOM	1463	O	ASN	A	711	16.336	37.991	5.230	1.00	51.44	O
ATOM	1464	N	TRP	A	712	18.147	39.036	6.052	1.00	46.43	N
ATOM	1465	CA	TRP	A	712	19.057	37.952	5.712	1.00	42.91	C
ATOM	1466	CB	TRP	A	712	20.506	38.436	5.704	1.00	39.68	C
ATOM	1467	CG	TRP	A	712	20.906	38.997	4.395	1.00	37.68	C
ATOM	1468	CD2	TRP	A	712	20.793	38.354	3.119	1.00	36.30	C
ATOM	1469	CE2	TRP	A	712	21.270	39.260	2.156	1.00	36.03	C
ATOM	1470	CE3	TRP	A	712	20.334	37.098	2.698	1.00	36.25	C
ATOM	1471	CD1	TRP	A	712	21.435	40.229	4.161	1.00	37.00	C
ATOM	1472	NE1	TRP	A	712	21.656	40.396	2.818	1.00	37.53	N
ATOM	1473	CZ2	TRP	A	712	21.300	38.953	0.791	1.00	35.36	C
ATOM	1474	CZ3	TRP	A	712	20.366	36.791	1.343	1.00	34.90	C
ATOM	1475	CH2	TRP	A	712	20.846	37.716	0.406	1.00	34.68	C
ATOM	1476	C	TRP	A	712	18.907	36.842	6.732	1.00	42.51	C
ATOM	1477	O	TRP	A	712	18.891	35.662	6.392	1.00	43.40	O
ATOM	1478	N	GLN	A	713	18.807	37.231	7.994	1.00	41.07	N
ATOM	1479	CA	GLN	A	713	18.640	36.259	9.055	1.00	38.78	C
ATOM	1480	CB	GLN	A	713	18.555	36.968	10.394	1.00	43.12	C
ATOM	1481	CG	GLN	A	713	18.818	36.075	11.599	1.00	50.56	C
ATOM	1482	CD	GLN	A	713	20.085	35.208	11.456	1.00	55.94	C
ATOM	1483	OE1	GLN	A	713	21.006	35.536	10.692	1.00	58.36	O
ATOM	1484	NE2	GLN	A	713	20.137	34.111	12.202	1.00	55.63	N
ATOM	1485	C	GLN	A	713	17.344	35.527	8.762	1.00	35.32	C
ATOM	1486	O	GLN	A	713	17.255	34.315	8.936	1.00	33.60	O
ATOM	1487	N	ARG	A	714	16.342	36.270	8.301	1.00	31.78	N
ATOM	1488	CA	ARG	A	714	15.051	35.681	7.995	1.00	29.47	C
ATOM	1489	CB	ARG	A	714	14.000	36.766	7.771	1.00	26.76	C
ATOM	1490	CG	ARG	A	714	12.621	36.184	7.586	1.00	24.13	C
ATOM	1491	CD	ARG	A	714	11.539	37.235	7.616	1.00	23.66	C
ATOM	1492	NE	ARG	A	714	10.214	36.621	7.589	1.00	21.91	N
ATOM	1493	CZ	ARG	A	714	9.702	35.903	8.585	1.00	21.33	C
ATOM	1494	NH1	ARG	A	714	10.399	35.708	9.700	1.00	16.47	N
ATOM	1495	NH2	ARG	A	714	8.496	35.364	8.455	1.00	23.12	N
ATOM	1496	C	ARG	A	714	15.141	34.793	6.762	1.00	28.68	C
ATOM	1497	O	ARG	A	714	14.460	33.766	6.668	1.00	27.60	O
ATOM	1498	N	PHE	A	715	15.981	35.195	5.814	1.00	27.84	N
ATOM	1499	CA	PHE	A	715	16.168	34.425	4.597	1.00	26.96	C
ATOM	1500	CB	PHE	A	715	17.117	35.143	3.645	1.00	25.94	C
ATOM	1501	CG	PHE	A	715	17.391	34.375	2.382	1.00	26.27	C
ATOM	1502	CD1	PHE	A	715	16.375	34.154	1.454	1.00	24.56	C
ATOM	1503	CD2	PHE	A	715	18.662	33.857	2.124	1.00	25.16	C
ATOM	1504	CE1	PHE	A	715	16.623	33.423	0.278	1.00	26.09	C
ATOM	1505	CE2	PHE	A	715	18.917	33.126	0.955	1.00	25.54	C
ATOM	1506	CZ	PHE	A	715	17.895	32.909	0.029	1.00	23.41	C
ATOM	1507	C	PHE	A	715	16.750	33.074	4.975	1.00	27.29	C
ATOM	1508	O	PHE	A	715	16.454	32.053	4.351	1.00	27.72	O
ATOM	1509	N	TYR	A	716	17.578	33.081	6.010	1.00	27.10	N
ATOM	1510	CA	TYR	A	716	18.200	31.866	6.504	1.00	28.86	C
ATOM	1511	CB	TYR	A	716	19.362	32.229	7.434	1.00	29.32	C
ATOM	1512	CG	TYR	A	716	20.081	31.051	8.048	1.00	32.16	C
ATOM	1513	CD1	TYR	A	716	19.534	30.352	9.124	1.00	32.43	C
ATOM	1514	CE1	TYR	A	716	20.208	29.272	9.698	1.00	35.06	C

ATOM	1515	CD2	TYR	A	716	21.322	30.640	7.560	1.00	33.66	C
ATOM	1516	CE2	TYR	A	716	22.004	29.565	8.124	1.00	34.94	C
ATOM	1517	CZ	TYR	A	716	21.444	28.884	9.189	1.00	36.33	C
ATOM	1518	OH	TYR	A	716	22.116	27.807	9.727	1.00	38.02	O
ATOM	1519	C	TYR	A	716	17.164	31.018	7.244	1.00	29.13	C
ATOM	1520	O	TYR	A	716	17.142	29.801	7.096	1.00	31.03	O
ATOM	1521	N	GLN	A	717	16.312	31.663	8.039	1.00	28.67	N
ATOM	1522	CA	GLN	A	717	15.280	30.955	8.795	1.00	28.75	C
ATOM	1523	CB	GLN	A	717	14.569	31.907	9.760	1.00	29.50	C
ATOM	1524	CG	GLN	A	717	15.473	32.513	10.821	1.00	35.28	C
ATOM	1525	CD	GLN	A	717	14.723	33.450	11.772	1.00	39.40	C
ATOM	1526	OE1	GLN	A	717	14.199	34.506	11.371	1.00	39.87	O
ATOM	1527	NE2	GLN	A	717	14.666	33.061	13.043	1.00	41.33	N
ATOM	1528	C	GLN	A	717	14.245	30.323	7.862	1.00	27.89	C
ATOM	1529	O	GLN	A	717	13.829	29.189	8.069	1.00	27.43	O
ATOM	1530	N	LEU	A	718	13.833	31.061	6.838	1.00	25.98	N
ATOM	1531	CA	LEU	A	718	12.857	30.551	5.889	1.00	25.25	C
ATOM	1532	CB	LEU	A	718	12.286	31.705	5.056	1.00	23.28	C
ATOM	1533	CG	LEU	A	718	11.584	32.812	5.858	1.00	23.59	C
ATOM	1534	CD1	LEU	A	718	10.896	33.760	4.901	1.00	23.47	C
ATOM	1535	CD2	LEU	A	718	10.561	32.212	6.830	1.00	22.06	C
ATOM	1536	C	LEU	A	718	13.435	29.455	4.980	1.00	26.33	C
ATOM	1537	O	LEU	A	718	12.765	28.443	4.731	1.00	27.82	O
ATOM	1538	N	THR	A	719	14.664	29.635	4.489	1.00	24.86	N
ATOM	1539	CA	THR	A	719	15.275	28.615	3.631	1.00	24.23	C
ATOM	1540	CB	THR	A	719	16.593	29.113	2.944	1.00	23.05	C
ATOM	1541	OG1	THR	A	719	17.495	29.649	3.922	1.00	24.18	O
ATOM	1542	CG2	THR	A	719	16.276	30.175	1.898	1.00	21.38	C
ATOM	1543	C	THR	A	719	15.563	27.355	4.452	1.00	24.68	C
ATOM	1544	O	THR	A	719	15.558	26.235	3.926	1.00	23.31	O
ATOM	1545	N	LYS	A	720	15.811	27.545	5.746	1.00	25.26	N
ATOM	1546	CA	LYS	A	720	16.057	26.429	6.650	1.00	25.39	C
ATOM	1547	CB	LYS	A	720	16.475	26.953	8.021	1.00	27.88	C
ATOM	1548	CG	LYS	A	720	17.985	26.951	8.261	1.00	35.07	C
ATOM	1549	CD	LYS	A	720	18.487	25.526	8.510	1.00	39.58	C
ATOM	1550	CE	LYS	A	720	19.987	25.486	8.777	1.00	41.66	C
ATOM	1551	NZ	LYS	A	720	20.466	24.101	9.077	1.00	42.32	N
ATOM	1552	C	LYS	A	720	14.764	25.609	6.761	1.00	24.59	C
ATOM	1553	O	LYS	A	720	14.784	24.379	6.702	1.00	24.95	O
ATOM	1554	N	LEU	A	721	13.635	26.297	6.898	1.00	22.78	N
ATOM	1555	CA	LEU	A	721	12.352	25.623	7.000	1.00	21.27	C
ATOM	1556	CB	LEU	A	721	11.228	26.641	7.212	1.00	17.24	C
ATOM	1557	CG	LEU	A	721	9.811	26.041	7.225	1.00	17.24	C
ATOM	1558	CD1	LEU	A	721	9.700	24.961	8.310	1.00	10.42	C
ATOM	1559	CD2	LEU	A	721	8.784	27.149	7.433	1.00	14.20	C
ATOM	1560	C	LEU	A	721	12.085	24.797	5.739	1.00	21.96	C
ATOM	1561	O	LEU	A	721	11.668	23.643	5.830	1.00	22.78	O
ATOM	1562	N	LEU	A	722	12.316	25.385	4.567	1.00	20.84	N
ATOM	1563	CA	LEU	A	722	12.110	24.661	3.315	1.00	19.20	C
ATOM	1564	CB	LEU	A	722	12.528	25.523	2.119	1.00	18.43	C
ATOM	1565	CG	LEU	A	722	11.665	26.766	1.865	1.00	18.22	C
ATOM	1566	CD1	LEU	A	722	12.195	27.539	0.667	1.00	15.79	C
ATOM	1567	CD2	LEU	A	722	10.213	26.333	1.614	1.00	18.71	C
ATOM	1568	C	LEU	A	722	12.907	23.356	3.333	1.00	19.29	C
ATOM	1569	O	LEU	A	722	12.369	22.293	3.025	1.00	21.96	O
ATOM	1570	N	ASP	A	723	14.181	23.430	3.700	1.00	17.90	N
ATOM	1571	CA	ASP	A	723	15.016	22.235	3.769	1.00	19.33	C
ATOM	1572	CB	ASP	A	723	16.394	22.567	4.341	1.00	19.49	C
ATOM	1573	CG	ASP	A	723	17.305	23.269	3.346	1.00	23.73	C
ATOM	1574	OD1	ASP	A	723	16.839	23.680	2.254	1.00	23.02	O
ATOM	1575	OD2	ASP	A	723	18.504	23.410	3.677	1.00	23.24	O
ATOM	1576	C	ASP	A	723	14.395	21.140	4.647	1.00	21.50	C
ATOM	1577	O	ASP	A	723	14.368	19.962	4.259	1.00	21.79	O
ATOM	1578	N	SER	A	724	13.905	21.529	5.826	1.00	21.28	N
ATOM	1579	CA	SER	A	724	13.324	20.580	6.767	1.00	21.43	C
ATOM	1580	CB	SER	A	724	12.933	21.279	8.081	1.00	24.25	C

ATOM	1581	OG	SER	A 724	11.953	22.284	7.891	1.00	30.59	O
ATOM	1582	C	SER	A 724	12.138	19.828	6.190	1.00	21.15	C
ATOM	1583	O	SER	A 724	11.824	18.719	6.631	1.00	20.68	O
ATOM	1584	N	MET	A 725	11.492	20.411	5.185	1.00	20.81	N
ATOM	1585	CA	MET	A 725	10.359	19.744	4.557	1.00	19.28	C
ATOM	1586	CB	MET	A 725	9.784	20.612	3.438	1.00	17.21	C
ATOM	1587	CG	MET	A 725	9.088	21.875	3.958	1.00	17.72	C
ATOM	1588	SD	MET	A 725	7.756	21.536	5.174	1.00	18.39	S
ATOM	1589	CE	MET	A 725	6.758	20.309	4.274	1.00	16.17	C
ATOM	1590	C	MET	A 725	10.791	18.380	4.015	1.00	18.66	C
ATOM	1591	O	MET	A 725	9.990	17.433	3.972	1.00	18.08	O
ATOM	1592	N	HIS	A 726	12.060	18.275	3.622	1.00	17.15	N
ATOM	1593	CA	HIS	A 726	12.594	17.015	3.100	1.00	18.01	C
ATOM	1594	CB	HIS	A 726	14.058	17.168	2.683	1.00	17.04	C
ATOM	1595	CG	HIS	A 726	14.240	17.744	1.317	1.00	16.42	C
ATOM	1596	CD2	HIS	A 726	14.997	18.778	0.879	1.00	15.93	C
ATOM	1597	ND1	HIS	A 726	13.603	17.236	0.205	1.00	15.81	N
ATOM	1598	CE1	HIS	A 726	13.959	17.933	-0.859	1.00	16.01	C
ATOM	1599	NE2	HIS	A 726	14.806	18.873	-0.477	1.00	16.64	N
ATOM	1600	C	HIS	A 726	12.502	15.912	4.139	1.00	18.05	C
ATOM	1601	O	HIS	A 726	12.198	14.773	3.814	1.00	18.66	O
ATOM	1602	N	GLU	A 727	12.768	16.272	5.391	1.00	20.56	N
ATOM	1603	CA	GLU	A 727	12.728	15.328	6.499	1.00	22.84	C
ATOM	1604	CB	GLU	A 727	13.481	15.893	7.692	1.00	22.48	C
ATOM	1605	CG	GLU	A 727	13.963	14.825	8.620	1.00	24.12	C
ATOM	1606	CD	GLU	A 727	14.630	15.392	9.846	1.00	29.38	C
ATOM	1607	OE1	GLU	A 727	15.395	16.380	9.704	1.00	31.41	O
ATOM	1608	OE2	GLU	A 727	14.396	14.837	10.945	1.00	28.96	O
ATOM	1609	C	GLU	A 727	11.292	15.025	6.905	1.00	23.99	C
ATOM	1610	O	GLU	A 727	10.976	13.904	7.304	1.00	25.80	O
ATOM	1611	N	VAL	A 728	10.428	16.031	6.824	1.00	23.70	N
ATOM	1612	CA	VAL	A 728	9.028	15.827	7.153	1.00	24.40	C
ATOM	1613	CB	VAL	A 728	8.234	17.142	7.040	1.00	24.48	C
ATOM	1614	CG1	VAL	A 728	6.744	16.875	7.249	1.00	24.28	C
ATOM	1615	CG2	VAL	A 728	8.756	18.144	8.070	1.00	22.75	C
ATOM	1616	C	VAL	A 728	8.474	14.804	6.163	1.00	25.55	C
ATOM	1617	O	VAL	A 728	7.863	13.811	6.562	1.00	25.65	O
ATOM	1618	N	VAL	A 729	8.711	15.046	4.872	1.00	25.02	N
ATOM	1619	CA	VAL	A 729	8.252	14.148	3.816	1.00	24.40	C
ATOM	1620	CB	VAL	A 729	8.672	14.674	2.405	1.00	24.45	C
ATOM	1621	CG1	VAL	A 729	8.302	13.664	1.327	1.00	22.33	C
ATOM	1622	CG2	VAL	A 729	7.974	16.004	2.115	1.00	24.92	C
ATOM	1623	C	VAL	A 729	8.791	12.727	4.028	1.00	24.66	C
ATOM	1624	O	VAL	A 729	8.054	11.750	3.881	1.00	25.19	O
ATOM	1625	N	GLU	A 730	10.069	12.609	4.377	1.00	25.70	N
ATOM	1626	CA	GLU	A 730	10.684	11.302	4.615	1.00	26.92	C
ATOM	1627	CB	GLU	A 730	12.110	11.505	5.127	1.00	30.97	C
ATOM	1628	CG	GLU	A 730	12.924	10.220	5.202	1.00	39.85	C
ATOM	1629	CD	GLU	A 730	14.322	10.424	5.784	1.00	44.69	C
ATOM	1630	OE1	GLU	A 730	14.767	11.596	5.917	1.00	45.55	O
ATOM	1631	OE2	GLU	A 730	14.977	9.397	6.091	1.00	48.01	O
ATOM	1632	C	GLU	A 730	9.876	10.440	5.622	1.00	26.45	C
ATOM	1633	O	GLU	A 730	9.757	9.218	5.468	1.00	24.63	O
ATOM	1634	N	ASN	A 731	9.320	11.096	6.637	1.00	23.97	N
ATOM	1635	CA	ASN	A 731	8.512	10.450	7.666	1.00	22.40	C
ATOM	1636	CB	ASN	A 731	8.365	11.389	8.859	1.00	23.25	C
ATOM	1637	CG	ASN	A 731	9.618	11.463	9.693	1.00	26.42	C
ATOM	1638	OD1	ASN	A 731	9.931	10.527	10.435	1.00	28.31	O
ATOM	1639	ND2	ASN	A 731	10.353	12.568	9.576	1.00	25.72	N
ATOM	1640	C	ASN	A 731	7.120	10.041	7.202	1.00	21.17	C
ATOM	1641	O	ASN	A 731	6.633	8.962	7.542	1.00	19.90	O
ATOM	1642	N	LEU	A 732	6.478	10.926	6.445	1.00	21.84	N
ATOM	1643	CA	LEU	A 732	5.128	10.704	5.933	1.00	20.77	C
ATOM	1644	CB	LEU	A 732	4.594	12.002	5.345	1.00	21.46	C
ATOM	1645	CG	LEU	A 732	4.620	13.162	6.333	1.00	22.65	C
ATOM	1646	CD1	LEU	A 732	4.136	14.434	5.632	1.00	20.86	C

ATOM	1647	CD2	LEU	A	732	3.742	12.812	7.546	1.00	19.65	C
ATOM	1648	C	LEU	A	732	5.060	9.604	4.877	1.00	21.08	C
ATOM	1649	O	LEU	A	732	4.022	8.965	4.704	1.00	19.47	O
ATOM	1650	N	LEU	A	733	6.168	9.388	4.172	1.00	21.05	N
ATOM	1651	CA	LEU	A	733	6.221	8.362	3.137	1.00	22.10	C
ATOM	1652	CB	LEU	A	733	7.391	8.616	2.184	1.00	21.78	C
ATOM	1653	CG	LEU	A	733	7.340	9.922	1.382	1.00	22.39	C
ATOM	1654	CD1	LEU	A	733	8.593	10.050	0.522	1.00	23.05	C
ATOM	1655	CD2	LEU	A	733	6.091	9.933	0.523	1.00	21.13	C
ATOM	1656	C	LEU	A	733	6.352	6.973	3.728	1.00	22.69	C
ATOM	1657	O	LEU	A	733	6.176	5.982	3.030	1.00	23.30	O
ATOM	1658	N	ASN	A	734	6.663	6.903	5.017	1.00	22.52	N
ATOM	1659	CA	ASN	A	734	6.817	5.623	5.696	1.00	24.39	C
ATOM	1660	CB	ASN	A	734	7.716	5.788	6.921	1.00	22.11	C
ATOM	1661	CG	ASN	A	734	9.188	5.901	6.549	1.00	24.38	C
ATOM	1662	OD1	ASN	A	734	9.979	6.497	7.284	1.00	25.50	O
ATOM	1663	ND2	ASN	A	734	9.564	5.323	5.408	1.00	21.41	N
ATOM	1664	C	ASN	A	734	5.474	5.037	6.121	1.00	26.57	C
ATOM	1665	O	ASN	A	734	5.411	3.922	6.653	1.00	26.02	O
ATOM	1666	N	TYR	A	735	4.399	5.784	5.887	1.00	25.48	N
ATOM	1667	CA	TYR	A	735	3.089	5.302	6.273	1.00	26.47	C
ATOM	1668	CB	TYR	A	735	2.208	6.473	6.727	1.00	28.08	C
ATOM	1669	CG	TYR	A	735	2.728	7.110	7.998	1.00	30.37	C
ATOM	1670	CD1	TYR	A	735	3.453	8.303	7.965	1.00	30.38	C
ATOM	1671	CE1	TYR	A	735	4.020	8.831	9.121	1.00	31.54	C
ATOM	1672	CD2	TYR	A	735	2.579	6.466	9.230	1.00	29.34	C
ATOM	1673	CE2	TYR	A	735	3.145	6.986	10.387	1.00	30.80	C
ATOM	1674	CZ	TYR	A	735	3.866	8.164	10.327	1.00	32.07	C
ATOM	1675	OH	TYR	A	735	4.463	8.659	11.469	1.00	35.32	O
ATOM	1676	C	TYR	A	735	2.414	4.485	5.183	1.00	27.80	C
ATOM	1677	O	TYR	A	735	2.763	4.575	3.996	1.00	26.56	O
ATOM	1678	N	CYS	A	736	1.450	3.673	5.609	1.00	27.77	N
ATOM	1679	CA	CYS	A	736	0.730	2.788	4.712	1.00	28.48	C
ATOM	1680	CB	CYS	A	736	-0.232	1.895	5.495	1.00	29.54	C
ATOM	1681	SG	CYS	A	736	-1.077	0.675	4.454	1.00	33.33	S
ATOM	1682	C	CYS	A	736	-0.044	3.529	3.654	1.00	28.99	C
ATOM	1683	O	CYS	A	736	-0.900	4.361	3.958	1.00	30.75	O
ATOM	1684	N	PHE	A	737	0.257	3.209	2.402	1.00	27.64	N
ATOM	1685	CA	PHE	A	737	-0.424	3.841	1.288	1.00	28.07	C
ATOM	1686	CB	PHE	A	737	0.461	3.820	0.049	1.00	29.51	C
ATOM	1687	CG	PHE	A	737	-0.276	4.156	-1.215	1.00	31.81	C
ATOM	1688	CD1	PHE	A	737	-0.915	5.385	-1.360	1.00	32.37	C
ATOM	1689	CD2	PHE	A	737	-0.347	3.236	-2.258	1.00	32.43	C
ATOM	1690	CE1	PHE	A	737	-1.615	5.697	-2.530	1.00	33.33	C
ATOM	1691	CE2	PHE	A	737	-1.047	3.540	-3.436	1.00	33.88	C
ATOM	1692	CZ	PHE	A	737	-1.679	4.772	-3.570	1.00	32.10	C
ATOM	1693	C	PHE	A	737	-1.747	3.140	1.002	1.00	27.87	C
ATOM	1694	O	PHE	A	737	-2.763	3.799	0.771	1.00	27.51	O
ATOM	1695	N	GLN	A	738	-1.715	1.811	1.004	1.00	26.66	N
ATOM	1696	CA	GLN	A	738	-2.911	1.031	0.748	1.00	27.90	C
ATOM	1697	CB	GLN	A	738	-3.191	0.925	-0.767	1.00	28.34	C
ATOM	1698	CG	GLN	A	738	-2.168	0.121	-1.538	1.00	29.15	C
ATOM	1699	CD	GLN	A	738	-2.483	-0.022	-3.021	1.00	28.82	C
ATOM	1700	OE1	GLN	A	738	-1.592	-0.298	-3.822	1.00	32.21	O
ATOM	1701	NE2	GLN	A	738	-3.745	0.155	-3.389	1.00	28.71	N
ATOM	1702	C	GLN	A	738	-2.841	-0.391	1.332	1.00	28.35	C
ATOM	1703	O	GLN	A	738	-1.763	-0.957	1.569	1.00	30.41	O
ATOM	1704	N	THR	A	739	-4.029	-0.932	1.530	1.00	27.32	N
ATOM	1705	CA	THR	A	739	-4.261	-2.234	2.048	1.00	27.03	C
ATOM	1706	CB	THR	A	739	-5.652	-2.203	2.720	1.00	26.21	C
ATOM	1707	OG1	THR	A	739	-5.504	-2.169	4.151	1.00	28.10	O
ATOM	1708	CG2	THR	A	739	-6.482	-3.371	2.267	1.00	25.04	C
ATOM	1709	C	THR	A	739	-4.146	-3.290	0.935	1.00	28.52	C
ATOM	1710	O	THR	A	739	-4.088	-2.931	-0.236	1.00	27.95	O
ATOM	1711	N	PHE	A	740	-4.056	-4.567	1.306	1.00	28.47	N
ATOM	1712	CA	PHE	A	740	-4.000	-5.636	0.333	1.00	28.92	C

ATOM	1713	CB	PHE	A	740	-3.730	-6.986	1.002	1.00	28.60	C
ATOM	1714	CG	PHE	A	740	-2.275	-7.353	1.061	1.00	28.35	C
ATOM	1715	CD1	PHE	A	740	-1.443	-6.779	2.005	1.00	27.97	C
ATOM	1716	CD2	PHE	A	740	-1.724	-8.234	0.131	1.00	28.56	C
ATOM	1717	CE1	PHE	A	740	-0.085	-7.067	2.027	1.00	26.87	C
ATOM	1718	CE2	PHE	A	740	-0.359	-8.530	0.143	1.00	25.73	C
ATOM	1719	CZ	PHE	A	740	0.462	-7.940	1.096	1.00	25.29	C
ATOM	1720	C	PHE	A	740	-5.351	-5.690	-0.396	1.00	29.22	C
ATOM	1721	O	PHE	A	740	-5.400	-5.943	-1.589	1.00	28.56	O
ATOM	1722	N	LEU	A	741	-6.451	-5.465	0.319	1.00	30.16	N
ATOM	1723	CA	LEU	A	741	-7.772	-5.475	-0.305	1.00	31.41	C
ATOM	1724	CB	LEU	A	741	-8.854	-5.208	0.742	1.00	29.37	C
ATOM	1725	CG	LEU	A	741	-10.262	-5.734	0.455	1.00	29.03	C
ATOM	1726	CD1	LEU	A	741	-11.272	-4.961	1.316	1.00	24.58	C
ATOM	1727	CD2	LEU	A	741	-10.590	-5.575	-1.013	1.00	25.66	C
ATOM	1728	C	LEU	A	741	-7.830	-4.381	-1.385	1.00	34.12	C
ATOM	1729	O	LEU	A	741	-8.309	-4.631	-2.495	1.00	34.57	O
ATOM	1730	N	ASP	A	742	-7.330	-3.182	-1.060	1.00	36.41	N
ATOM	1731	CA	ASP	A	742	-7.312	-2.052	-1.998	1.00	39.05	C
ATOM	1732	CB	ASP	A	742	-6.699	-0.788	-1.367	1.00	41.59	C
ATOM	1733	CG	ASP	A	742	-7.447	-0.314	-0.130	1.00	44.91	C
ATOM	1734	OD1	ASP	A	742	-8.703	-0.337	-0.137	1.00	44.96	O
ATOM	1735	OD2	ASP	A	742	-6.770	0.097	0.844	1.00	44.33	O
ATOM	1736	C	ASP	A	742	-6.497	-2.383	-3.233	1.00	39.68	C
ATOM	1737	O	ASP	A	742	-6.851	-1.982	-4.341	1.00	39.59	O
ATOM	1738	N	LYS	A	743	-5.398	-3.105	-3.045	1.00	40.40	N
ATOM	1739	CA	LYS	A	743	-4.543	-3.469	-4.167	1.00	41.01	C
ATOM	1740	CB	LYS	A	743	-3.218	-4.043	-3.671	1.00	39.01	C
ATOM	1741	CG	LYS	A	743	-2.246	-4.390	-4.789	1.00	38.60	C
ATOM	1742	CD	LYS	A	743	-1.893	-3.168	-5.628	1.00	38.68	C
ATOM	1743	CE	LYS	A	743	-0.895	-3.523	-6.722	1.00	39.76	C
ATOM	1744	NZ	LYS	A	743	-0.575	-2.370	-7.611	1.00	39.51	N
ATOM	1745	C	LYS	A	743	-5.201	-4.470	-5.106	1.00	41.84	C
ATOM	1746	O	LYS	A	743	-5.292	-4.228	-6.311	1.00	42.58	O
ATOM	1747	N	THR	A	744	-5.658	-5.586	-4.547	1.00	43.57	N
ATOM	1748	CA	THR	A	744	-6.295	-6.653	-5.318	1.00	45.64	C
ATOM	1749	CB	THR	A	744	-6.836	-7.758	-4.392	1.00	44.98	C
ATOM	1750	CG1	THR	A	744	-5.747	-8.349	-3.675	1.00	44.07	O
ATOM	1751	CG2	THR	A	744	-7.546	-8.839	-5.206	1.00	45.66	C
ATOM	1752	C	THR	A	744	-7.432	-6.185	-6.212	1.00	47.40	C
ATOM	1753	O	THR	A	744	-7.654	-6.753	-7.280	1.00	47.75	O
ATOM	1754	N	MET	A	745	-8.154	-5.160	-5.773	1.00	49.80	N
ATOM	1755	CA	MET	A	745	-9.259	-4.629	-6.559	1.00	52.76	C
ATOM	1756	CB	MET	A	745	-10.380	-4.139	-5.649	1.00	54.50	C
ATOM	1757	CG	MET	A	745	-10.866	-5.160	-4.647	1.00	59.16	C
ATOM	1758	SD	MET	A	745	-12.395	-4.619	-3.844	1.00	66.09	S
ATOM	1759	CE	MET	A	745	-11.941	-2.945	-3.284	1.00	64.45	C
ATOM	1760	C	MET	A	745	-8.805	-3.476	-7.449	1.00	53.67	C
ATOM	1761	O	MET	A	745	-9.512	-3.095	-8.381	1.00	55.39	O
ATOM	1762	N	SER	A	746	-7.629	-2.922	-7.167	1.00	53.46	N
ATOM	1763	CA	SER	A	746	-7.107	-1.807	-7.956	1.00	54.81	C
ATOM	1764	CB	SER	A	746	-6.260	-0.874	-7.077	1.00	54.57	C
ATOM	1765	OG	SER	A	746	-7.059	-0.166	-6.137	1.00	58.74	O
ATOM	1766	C	SER	A	746	-6.267	-2.252	-9.151	1.00	54.77	C
ATOM	1767	O	SER	A	746	-5.656	-1.422	-9.827	1.00	55.13	O
ATOM	1768	N	ILE	A	747	-6.235	-3.552	-9.427	1.00	54.44	N
ATOM	1769	CA	ILE	A	747	-5.426	-4.034	-10.537	1.00	53.35	C
ATOM	1770	CB	ILE	A	747	-3.918	-3.842	-10.217	1.00	51.95	C
ATOM	1771	CG2	ILE	A	747	-3.430	-4.956	-9.307	1.00	50.58	C
ATOM	1772	CG1	ILE	A	747	-3.097	-3.826	-11.501	1.00	51.96	C
ATOM	1773	CD1	ILE	A	747	-1.639	-3.458	-11.276	1.00	53.37	C
ATOM	1774	C	ILE	A	747	-5.684	-5.502	-10.859	1.00	52.81	C
ATOM	1775	O	ILE	A	747	-5.964	-6.307	-9.969	1.00	53.50	O
ATOM	1776	N	GLU	A	748	-5.587	-5.835	-12.142	1.00	51.77	N
ATOM	1777	CA	GLU	A	748	-5.778	-7.204	-12.614	1.00	51.90	C
ATOM	1778	CB	GLU	A	748	-5.972	-7.217	-14.131	1.00	54.94	C

ATOM	1779	CG	GLU	A	748	-4.810	-6.566	-14.860	1.00	61.17	C
ATOM	1780	CD	GLU	A	748	-4.939	-6.627	-16.363	1.00	64.72	C
ATOM	1781	OE1	GLU	A	748	-6.006	-6.226	-16.882	1.00	66.54	O
ATOM	1782	OE2	GLU	A	748	-3.966	-7.066	-17.022	1.00	66.74	O
ATOM	1783	C	GLU	A	748	-4.527	-8.004	-12.256	1.00	49.12	C
ATOM	1784	O	GLU	A	748	-3.416	-7.465	-12.242	1.00	49.04	O
ATOM	1785	N	PHE	A	749	-4.708	-9.291	-11.991	1.00	45.70	N
ATOM	1786	CA	PHE	A	749	-3.601	-10.153	-11.609	1.00	43.81	C
ATOM	1787	CB	PHE	A	749	-4.093	-11.596	-11.468	1.00	41.95	C
ATOM	1788	CG	PHE	A	749	-3.156	-12.481	-10.698	1.00	39.45	C
ATOM	1789	CD1	PHE	A	749	-2.822	-12.181	-9.385	1.00	39.11	C
ATOM	1790	CD2	PHE	A	749	-2.613	-13.615	-11.282	1.00	39.11	C
ATOM	1791	CE1	PHE	A	749	-1.960	-13.000	-8.666	1.00	39.67	C
ATOM	1792	CE2	PHE	A	749	-1.752	-14.441	-10.572	1.00	39.69	C
ATOM	1793	CZ	PHE	A	749	-1.425	-14.132	-9.260	1.00	39.69	C
ATOM	1794	C	PHE	A	749	-2.367	-10.121	-12.522	1.00	42.67	C
ATOM	1795	O	PHE	A	749	-1.237	-10.151	-12.036	1.00	42.30	O
ATOM	1796	N	PRO	A	750	-2.562	-10.072	-13.850	1.00	42.69	N
ATOM	1797	CD	PRO	A	750	-3.821	-10.228	-14.599	1.00	42.04	C
ATOM	1798	CA	PRO	A	750	-1.413	-10.043	-14.769	1.00	42.15	C
ATOM	1799	CB	PRO	A	750	-2.077	-9.999	-16.143	1.00	42.26	C
ATOM	1800	CG	PRO	A	750	-3.336	-10.780	-15.921	1.00	41.75	C
ATOM	1801	C	PRO	A	750	-0.445	-8.874	-14.545	1.00	42.03	C
ATOM	1802	O	PRO	A	750	0.777	-9.065	-14.547	1.00	41.01	O
ATOM	1803	N	GLU	A	751	-0.992	-7.672	-14.359	1.00	42.10	N
ATOM	1804	CA	GLU	A	751	-0.181	-6.479	-14.122	1.00	41.80	C
ATOM	1805	CB	GLU	A	751	-1.051	-5.237	-14.004	1.00	45.60	C
ATOM	1806	CG	GLU	A	751	-1.863	-4.856	-15.212	1.00	50.76	C
ATOM	1807	CD	GLU	A	751	-2.606	-3.547	-14.971	1.00	53.59	C
ATOM	1808	OE1	GLU	A	751	-1.933	-2.499	-14.829	1.00	55.27	O
ATOM	1809	OE2	GLU	A	751	-3.856	-3.567	-14.904	1.00	54.76	O
ATOM	1810	C	GLU	A	751	0.577	-6.612	-12.812	1.00	40.35	C
ATOM	1811	O	GLU	A	751	1.742	-6.235	-12.710	1.00	39.57	O
ATOM	1812	N	MET	A	752	-0.111	-7.123	-11.799	1.00	38.08	N
ATOM	1813	CA	MET	A	752	0.482	-7.305	-10.485	1.00	36.50	C
ATOM	1814	CB	MET	A	752	-0.595	-7.724	-9.489	1.00	38.23	C
ATOM	1815	CG	MET	A	752	-0.112	-7.937	-8.071	1.00	42.16	C
ATOM	1816	SD	MET	A	752	-1.445	-7.665	-6.870	1.00	46.19	S
ATOM	1817	CE	MET	A	752	-2.793	-8.691	-7.530	1.00	45.95	C
ATOM	1818	C	MET	A	752	1.584	-8.346	-10.550	1.00	34.03	C
ATOM	1819	O	MET	A	752	2.563	-8.262	-9.820	1.00	32.78	O
ATOM	1820	N	LEU	A	753	1.425	-9.320	-11.440	1.00	33.01	N
ATOM	1821	CA	LEU	A	753	2.422	-10.373	-11.608	1.00	32.98	C
ATOM	1822	CB	LEU	A	753	1.899	-11.465	-12.541	1.00	31.89	C
ATOM	1823	CG	LEU	A	753	2.193	-12.888	-12.076	1.00	31.73	C
ATOM	1824	CD1	LEU	A	753	1.618	-13.097	-10.676	1.00	30.99	C
ATOM	1825	CD2	LEU	A	753	1.595	-13.877	-13.065	1.00	29.81	C
ATOM	1826	C	LEU	A	753	3.678	-9.756	-12.201	1.00	32.62	C
ATOM	1827	O	LEU	A	753	4.785	-10.018	-11.741	1.00	33.11	O
ATOM	1828	N	ALA	A	754	3.493	-8.933	-13.228	1.00	32.32	N
ATOM	1829	CA	ALA	A	754	4.605	-8.254	-13.874	1.00	30.99	C
ATOM	1830	CB	ALA	A	754	4.103	-7.475	-15.079	1.00	29.43	C
ATOM	1831	C	ALA	A	754	5.236	-7.308	-12.852	1.00	30.53	C
ATOM	1832	O	ALA	A	754	6.452	-7.145	-12.803	1.00	30.15	O
ATOM	1833	N	GLU	A	755	4.392	-6.691	-12.034	1.00	30.94	N
ATOM	1834	CA	GLU	A	755	4.849	-5.767	-11.001	1.00	33.21	C
ATOM	1835	CB	GLU	A	755	3.656	-5.166	-10.273	1.00	33.78	C
ATOM	1836	CG	GLU	A	755	3.448	-3.690	-10.523	1.00	34.33	C
ATOM	1837	CD	GLU	A	755	2.067	-3.233	-10.090	1.00	36.38	C
ATOM	1838	OE1	GLU	A	755	1.619	-3.636	-8.989	1.00	34.46	O
ATOM	1839	OE2	GLU	A	755	1.437	-2.468	-10.854	1.00	37.25	O
ATOM	1840	C	GLU	A	755	5.733	-6.475	-9.991	1.00	35.08	C
ATOM	1841	O	GLU	A	755	6.781	-5.964	-9.598	1.00	37.12	O
ATOM	1842	N	ILE	A	756	5.298	-7.654	-9.568	1.00	36.05	N
ATOM	1843	CA	ILE	A	756	6.047	-8.447	-8.609	1.00	37.46	C
ATOM	1844	CB	ILE	A	756	5.212	-9.694	-8.185	1.00	35.45	C

ATOM	1845	CG2	ILE	A	756	6.066	-10.679	-7.403	1.00	33.71	C
ATOM	1846	CG1	ILE	A	756	4.009	-9.228	-7.353	1.00	33.65	C
ATOM	1847	CD1	ILE	A	756	2.928	-10.264	-7.139	1.00	31.03	C
ATOM	1848	C	ILE	A	756	7.406	-8.855	-9.192	1.00	39.91	C
ATOM	1849	O	ILE	A	756	8.449	-8.606	-8.584	1.00	41.68	O
ATOM	1850	N	ILE	A	757	7.390	-9.461	-10.375	1.00	41.81	N
ATOM	1851	CA	ILE	A	757	8.619	-9.896	-11.034	1.00	44.35	C
ATOM	1852	CB	ILE	A	757	8.314	-10.434	-12.438	1.00	43.22	C
ATOM	1853	CG2	ILE	A	757	9.610	-10.724	-13.190	1.00	43.25	C
ATOM	1854	CG1	ILE	A	757	7.456	-11.692	-12.308	1.00	43.31	C
ATOM	1855	CD1	ILE	A	757	7.043	-12.304	-13.618	1.00	42.35	C
ATOM	1856	C	ILE	A	757	9.615	-8.749	-11.133	1.00	46.93	C
ATOM	1857	O	ILE	A	757	10.809	-8.924	-10.902	1.00	46.46	O
ATOM	1858	N	THR	A	758	9.109	-7.574	-11.487	1.00	50.20	N
ATOM	1859	CA	THR	A	758	9.932	-6.382	-11.592	1.00	53.74	C
ATOM	1860	CB	THR	A	758	9.231	-5.311	-12.457	1.00	54.40	C
ATOM	1861	OG1	THR	A	758	9.055	-5.820	-13.787	1.00	53.70	O
ATOM	1862	CG2	THR	A	758	10.052	-4.018	-12.502	1.00	54.91	C
ATOM	1863	C	THR	A	758	10.102	-5.869	-10.166	1.00	56.76	C
ATOM	1864	O	THR	A	758	9.394	-4.955	-9.737	1.00	57.99	O
ATOM	1865	N	ASN	A	759	11.028	-6.488	-9.434	1.00	59.55	N
ATOM	1866	CA	ASN	A	759	11.309	-6.137	-8.039	1.00	60.54	C
ATOM	1867	CB	ASN	A	759	12.815	-6.199	-7.779	1.00	61.23	C
ATOM	1868	CG	ASN	A	759	13.334	-7.618	-7.714	1.00	62.21	C
ATOM	1869	OD1	ASN	A	759	14.543	-7.851	-7.755	1.00	62.16	O
ATOM	1870	ND2	ASN	A	759	12.421	-8.580	-7.604	1.00	61.69	N
ATOM	1871	C	ASN	A	759	10.773	-4.771	-7.625	1.00	60.85	C
ATOM	1872	O	ASN	A	759	9.662	-4.665	-7.103	1.00	60.82	O
ATOM	1873	N	ASN	A	768	17.782	7.993	-9.526	1.00	42.10	N
ATOM	1874	CA	ASN	A	768	17.798	8.350	-8.114	1.00	42.43	C
ATOM	1875	CB	ASN	A	768	19.169	8.043	-7.520	1.00	44.48	C
ATOM	1876	CG	ASN	A	768	19.082	7.501	-6.116	1.00	46.42	C
ATOM	1877	OD1	ASN	A	768	20.073	7.483	-5.384	1.00	48.28	O
ATOM	1878	ND2	ASN	A	768	17.894	7.040	-5.732	1.00	47.49	N
ATOM	1879	C	ASN	A	768	17.478	9.841	-7.945	1.00	41.65	C
ATOM	1880	O	ASN	A	768	17.705	10.639	-8.860	1.00	41.30	O
ATOM	1881	N	ILE	A	769	16.971	10.212	-6.769	1.00	39.53	N
ATOM	1882	CA	ILE	A	769	16.590	11.599	-6.494	1.00	37.58	C
ATOM	1883	CB	ILE	A	769	15.302	11.668	-5.636	1.00	36.18	C
ATOM	1884	CG2	ILE	A	769	14.766	13.096	-5.610	1.00	36.43	C
ATOM	1885	CG1	ILE	A	769	14.237	10.735	-6.213	1.00	36.83	C
ATOM	1886	CD1	ILE	A	769	13.082	10.453	-5.258	1.00	36.20	C
ATOM	1887	C	ILE	A	769	17.650	12.435	-5.776	1.00	37.17	C
ATOM	1888	O	ILE	A	769	18.352	11.956	-4.879	1.00	38.10	O
ATOM	1889	N	LYS	A	770	17.748	13.698	-6.169	1.00	35.61	N
ATOM	1890	CA	LYS	A	770	18.685	14.619	-5.541	1.00	33.69	C
ATOM	1891	CB	LYS	A	770	19.528	15.322	-6.603	1.00	35.14	C
ATOM	1892	CG	LYS	A	770	20.472	16.357	-6.032	1.00	37.32	C
ATOM	1893	CD	LYS	A	770	21.177	17.126	-7.131	1.00	40.79	C
ATOM	1894	CE	LYS	A	770	22.085	18.206	-6.547	1.00	44.20	C
ATOM	1895	NZ	LYS	A	770	22.775	19.014	-7.601	1.00	44.96	N
ATOM	1896	C	LYS	A	770	17.892	15.659	-4.733	1.00	31.89	C
ATOM	1897	O	LYS	A	770	17.129	16.439	-5.299	1.00	29.17	O
ATOM	1898	N	LYS	A	771	18.070	15.658	-3.413	1.00	31.51	N
ATOM	1899	CA	LYS	A	771	17.371	16.600	-2.534	1.00	30.94	C
ATOM	1900	CB	LYS	A	771	17.429	16.134	-1.078	1.00	31.94	C
ATOM	1901	CG	LYS	A	771	17.188	14.650	-0.840	1.00	35.14	C
ATOM	1902	CD	LYS	A	771	15.724	14.280	-0.952	1.00	36.76	C
ATOM	1903	CE	LYS	A	771	15.471	12.885	-0.374	1.00	37.96	C
ATOM	1904	NZ	LYS	A	771	15.670	12.836	1.105	1.00	39.47	N
ATOM	1905	C	LYS	A	771	18.062	17.950	-2.604	1.00	30.30	C
ATOM	1906	O	LYS	A	771	19.175	18.091	-2.103	1.00	32.14	O
ATOM	1907	N	LEU	A	772	17.425	18.945	-3.210	1.00	28.13	N
ATOM	1908	CA	LEU	A	772	18.045	20.261	-3.280	1.00	27.81	C
ATOM	1909	CB	LEU	A	772	17.360	21.117	-4.347	1.00	27.10	C
ATOM	1910	CG	LEU	A	772	17.483	20.570	-5.775	1.00	27.41	C

ATOM	1911	CD1	LEU	A	772	16.690	21.444	-6.729	1.00	26.45	C
ATOM	1912	CD2	LEU	A	772	18.947	20.523	-6.193	1.00	26.36	C
ATOM	1913	C	LEU	A	772	17.954	20.919	-1.898	1.00	28.16	C
ATOM	1914	O	LEU	A	772	16.887	20.917	-1.270	1.00	28.07	O
ATOM	1915	N	LEU	A	773	19.084	21.457	-1.431	1.00	27.54	N
ATOM	1916	CA	LEU	A	773	19.185	22.100	-0.118	1.00	27.61	C
ATOM	1917	CB	LEU	A	773	20.014	21.244	0.832	1.00	22.94	C
ATOM	1918	CG	LEU	A	773	19.632	19.829	1.232	1.00	23.69	C
ATOM	1919	CD1	LEU	A	773	20.844	19.157	1.862	1.00	18.12	C
ATOM	1920	CD2	LEU	A	773	18.456	19.862	2.199	1.00	22.12	C
ATOM	1921	C	LEU	A	773	19.864	23.470	-0.162	1.00	29.74	C
ATOM	1922	O	LEU	A	773	20.782	23.693	-0.951	1.00	29.86	O
ATOM	1923	N	PHE	A	774	19.426	24.371	0.717	1.00	30.73	N
ATOM	1924	CA	PHE	A	774	20.028	25.694	0.819	1.00	29.86	C
ATOM	1925	CB	PHE	A	774	19.001	26.739	1.278	1.00	28.70	C
ATOM	1926	CG	PHE	A	774	17.897	27.001	0.284	1.00	27.54	C
ATOM	1927	CD1	PHE	A	774	16.740	26.217	0.277	1.00	26.23	C
ATOM	1928	CD2	PHE	A	774	18.006	28.041	-0.640	1.00	26.58	C
ATOM	1929	CE1	PHE	A	774	15.707	26.460	-0.631	1.00	24.45	C
ATOM	1930	CE2	PHE	A	774	16.971	28.298	-1.560	1.00	26.65	C
ATOM	1931	CZ	PHE	A	774	15.820	27.502	-1.552	1.00	25.59	C
ATOM	1932	C	PHE	A	774	21.162	25.630	1.846	1.00	30.75	C
ATOM	1933	O	PHE	A	774	22.162	26.330	1.713	1.00	31.84	O
ATOM	1934	N	HIS	A	775	20.999	24.788	2.867	1.00	32.46	N
ATOM	1935	CA	HIS	A	775	21.996	24.638	3.927	1.00	34.79	C
ATOM	1936	CB	HIS	A	775	21.427	25.120	5.257	1.00	33.07	C
ATOM	1937	CG	HIS	A	775	20.709	26.428	5.167	1.00	33.70	C
ATOM	1938	CD2	HIS	A	775	19.388	26.724	5.215	1.00	33.95	C
ATOM	1939	ND1	HIS	A	775	21.362	27.624	4.966	1.00	34.26	N
ATOM	1940	CE1	HIS	A	775	20.474	28.601	4.891	1.00	35.29	C
ATOM	1941	NE2	HIS	A	775	19.269	28.081	5.037	1.00	34.15	N
ATOM	1942	C	HIS	A	775	22.417	23.185	4.080	1.00	37.89	C
ATOM	1943	O	HIS	A	775	21.577	22.293	4.147	1.00	40.08	O
ATOM	1944	N	GLN	A	776	23.719	22.944	4.159	1.00	42.42	N
ATOM	1945	CA	GLN	A	776	24.227	21.581	4.310	1.00	45.17	C
ATOM	1946	CB	GLN	A	776	25.664	21.501	3.791	1.00	46.91	C
ATOM	1947	CG	GLN	A	776	25.998	22.538	2.720	1.00	49.96	C
ATOM	1948	CD	GLN	A	776	24.979	22.582	1.595	1.00	50.90	C
ATOM	1949	OE1	GLN	A	776	24.747	21.583	0.908	1.00	51.71	O
ATOM	1950	NE2	GLN	A	776	24.366	23.747	1.401	1.00	51.49	N
ATOM	1951	C	GLN	A	776	24.187	21.145	5.778	1.00	45.57	C
ATOM	1952	O	GLN	A	776	24.275	21.978	6.690	1.00	45.48	O
ATOM	1953	C1	486	A	800	-4.958	16.449	3.385	1.00	27.18	C
ATOM	1954	C2	486	A	800	-3.921	17.579	3.147	1.00	28.10	C
ATOM	1955	C3	486	A	800	-2.450	17.212	3.275	1.00	27.60	C
ATOM	1956	C4	486	A	800	-1.994	15.955	3.393	1.00	26.39	C
ATOM	1957	C5	486	A	800	-2.905	14.788	3.360	1.00	26.71	C
ATOM	1958	C6	486	A	800	-4.454	15.014	3.103	1.00	26.77	C
ATOM	1959	C7	486	A	800	-0.433	15.812	3.567	1.00	25.90	C
ATOM	1960	C8	486	A	800	-0.189	14.649	4.483	1.00	27.23	C
ATOM	1961	C9	486	A	800	-0.833	13.349	3.908	1.00	25.77	C
ATOM	1962	C10	486	A	800	-2.410	13.501	3.556	1.00	25.96	C
ATOM	1963	C11	486	A	800	-0.571	12.327	5.059	1.00	25.42	C
ATOM	1964	C12	486	A	800	-1.124	10.917	4.855	1.00	27.24	C
ATOM	1965	C13	486	A	800	-2.720	11.198	4.703	1.00	26.46	C
ATOM	1966	C14	486	A	800	-3.256	12.075	3.527	1.00	25.78	C
ATOM	1967	C15	486	A	800	0.907	12.024	5.562	1.00	25.35	C
ATOM	1968	C16	486	A	800	0.785	10.627	6.286	1.00	25.11	C
ATOM	1969	C17	486	A	800	-0.701	10.124	6.183	1.00	26.20	C
ATOM	1970	O3	486	A	800	-0.673	8.694	6.061	1.00	28.33	O
ATOM	1971	C18	486	A	800	-3.160	11.380	2.078	1.00	27.13	C
ATOM	1972	C19	486	A	800	-0.508	10.116	3.610	1.00	26.07	C
ATOM	1973	C22	486	A	800	-2.424	12.015	0.979	1.00	24.15	C
ATOM	1974	C23	486	A	800	-2.301	11.476	-0.327	1.00	23.04	C
ATOM	1975	C24	486	A	800	-2.912	10.208	-0.686	1.00	21.19	C
ATOM	1976	C25	486	A	800	-3.668	9.523	0.414	1.00	24.27	C

ATOM	1977	C26	486	A	800	-3.784	10.100	1.744	1.00	25.14	C
ATOM	1978	N27	486	A	800	-2.840	9.596	-2.012	1.00	19.86	N
ATOM	1979	C28	486	A	800	-2.092	10.334	-3.057	1.00	20.73	C
ATOM	1980	C29	486	A	800	-4.180	9.302	-2.551	1.00	22.81	C
ATOM	1981	O30	486	A	800	-4.290	18.735	2.915	1.00	32.03	O
ATOM	1982	C30	486	A	800	-2.243	10.906	8.320	1.00	23.29	C
ATOM	1983	C31	486	A	800	-1.498	10.490	7.421	1.00	25.04	C
ATOM	1984	C32	486	A	800	-3.042	11.470	9.451	1.00	19.34	C
ATOM	1985	O01	HXD	A	901	-6.962	21.669	-1.158	1.00	40.34	O
ATOM	1986	C02	HXD	A	901	-6.160	21.132	-2.215	1.00	37.10	C
ATOM	1987	C03	HXD	A	901	-4.675	21.201	-1.830	1.00	35.54	C
ATOM	1988	C04	HXD	A	901	-3.977	22.305	-2.609	1.00	33.89	C
ATOM	1989	C05	HXD	A	901	-2.492	22.415	-2.281	1.00	29.78	C
ATOM	1990	C06	HXD	A	901	-1.703	22.581	-3.573	1.00	28.47	C
ATOM	1991	C07	HXD	A	901	-0.207	22.706	-3.342	1.00	29.00	C
ATOM	1992	O08	HXD	A	901	0.234	23.950	-3.865	1.00	26.97	O
ATOM	1993	O01	HXD	A	902	5.824	13.089	-3.330	1.00	34.85	O
ATOM	1994	C02	HXD	A	902	6.518	11.833	-3.324	1.00	38.64	C
ATOM	1995	C03	HXD	A	902	7.813	11.971	-2.525	1.00	38.20	C
ATOM	1996	C04	HXD	A	902	9.066	11.789	-3.388	1.00	40.00	C
ATOM	1997	C05	HXD	A	902	10.361	11.938	-2.554	1.00	41.48	C
ATOM	1998	C06	HXD	A	902	11.300	12.999	-3.154	1.00	43.04	C
ATOM	1999	C07	HXD	A	902	12.590	13.168	-2.355	1.00	42.99	C
ATOM	2000	O08	HXD	A	902	12.681	14.514	-1.894	1.00	44.45	O
ATOM	2001	O01	HXD	A	903	8.652	15.370	12.368	1.00	23.73	O
ATOM	2002	C02	HXD	A	903	8.980	16.106	11.195	1.00	26.20	C
ATOM	2003	C03	HXD	A	903	10.498	16.203	11.071	1.00	26.89	C
ATOM	2004	C04	HXD	A	903	11.039	17.441	11.767	1.00	31.18	C
ATOM	2005	C05	HXD	A	903	12.557	17.529	11.636	1.00	35.27	C
ATOM	2006	C06	HXD	A	903	12.982	18.908	11.151	1.00	38.80	C
ATOM	2007	C07	HXD	A	903	14.498	19.023	11.008	1.00	40.67	C
ATOM	2008	O08	HXD	A	903	14.960	20.059	11.858	1.00	41.11	O
ATOM	2009	O	HOH	A1001		0.264	29.631	-4.946	1.00	15.69	O
ATOM	2010	O	HOH	A1003		4.922	9.264	18.053	1.00	23.93	O
ATOM	2011	O	HOH	A1004		10.793	17.474	-3.662	1.00	22.83	O
ATOM	2012	O	HOH	A1006		-8.926	23.876	6.991	1.00	4.24	O
ATOM	2013	O	HOH	A1007		21.555	33.956	4.100	1.00	13.73	O
ATOM	2014	O	HOH	A1009		6.960	14.859	-1.622	1.00	29.61	O
ATOM	2015	O	HOH	A1010		10.525	18.968	0.100	1.00	20.63	O
ATOM	2016	O	HOH	A1011		12.358	13.474	1.582	1.00	34.18	O
ATOM	2017	O	HOH	A1012		-2.987	20.680	1.791	1.00	15.66	O
ATOM	2018	O	HOH	A1013		2.882	21.720	18.444	1.00	25.04	O
ATOM	2019	O	HOH	A1014		17.655	36.684	-2.546	1.00	20.06	O
ATOM	2020	O	HOH	A1015		2.631	28.765	-3.964	1.00	24.63	O
ATOM	2021	O	HOH	A1016		5.752	39.569	2.152	1.00	27.47	O
ATOM	2022	O	HOH	A1017		11.880	20.909	-19.991	1.00	20.93	O
ATOM	2023	O	HOH	A1018		-2.943	-1.298	-8.192	1.00	32.22	O
ATOM	2024	O	HOH	A1019		-2.182	6.572	4.843	1.00	45.22	O
ATOM	2025	O	HOH	A1020		10.994	18.677	-6.811	1.00	12.21	O
ATOM	2026	O	HOH	A1021		7.455	38.431	-3.850	1.00	25.68	O
TER	1		HOH	A1021							
END											

## CLAIMS

1. A crystal comprising at least 150 amino acid residues of the GR ligand binding domain.
2. A crystal according to claim 1 comprising the amino acid sequence from Leu-532 to Leu-732 of a human GR shown in Figure 7 or an amino acid sequence having at least 95% identity with the sequence and which encodes for a GR ligand binding domain.
3. A crystal according to claim 1 or claim 2 comprising an amino acid sequence from Leu-35 to Leu-235 of Seq ID No. 1.
4. A crystal according to any preceding claim comprising an amino acid sequence from Leu-14 to Leu-214 of Seq. ID No. 2.
5. A crystal according to any preceding claim comprising an amino acid sequence from Leu-35 to Leu-235 of Seq ID No. 3.
6. A crystal according to any one of claims 1 to 5 comprising the entire GR ligand binding domain.
7. A crystal according to any preceding claim produced using a sequence including helix 9 of GR.
8. A crystal according to any one of claims 1 to 7 usable in X-ray crystallography.
9. A crystal according to any one of claims 1 to 7 including a ligand bound to GR or a portion thereof.

10. A crystal according to claim 9, wherein the ligand is a GR antagonist.
11. A crystal according to claim 8 in which the ligand is RU-486 [(11 $\beta$ ,17 $\beta$ )-11-[4-(dimethylamino)phenyl]-17-hydroxy-17-(1-propynyl)-estra-4,9-dien-3-one, CAS registry number 84371-65-3], cortisol, dexamethasone or any other ligand that binds with high affinity (<100 nM to the internal GR binding cavity).
12. A crystal of GR LDB according to any preceding claim belonging to the space group P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub> and having the unit cell dimensions a = 67.33 Å, b = 87.4 Å, c = 93.11 Å,  $\alpha = \beta = \gamma = 90^\circ$ .
13. A crystal of GR LDB according to any preceding claim belonging to the space group P6<sub>5</sub> and having the unit cell dimensions a=b=132.1, c=53.  $\alpha = \beta = 90^\circ$ ,  $\gamma = 120^\circ$ .
14. A crystal of GR LDB according to any preceding claim belonging to the space group P2<sub>1</sub>2<sub>1</sub>2 and having the unit cell dimensions a= 74.5, b= 109.7, c= 39.1.  $\alpha = \beta = \gamma = 90^\circ$ .
15. A crystal of GR-LBD according to any one of claims 1 to 11 belonging to the space group P3; and having cell dimensions a=b=127.4, c=91.8,  $\alpha=\beta=90^\circ$ ,  $\gamma=120^\circ$ .
16. A crystal according to any of claims 1 to 15 having a resolution determined by X-ray crystallography of less than 3.6 Å.
17. A crystal according to claim 16 having a resolution determined by X-ray crystallography of less than 2.9 Å.
18. A machine-readable data storage medium, comprising a data storage material encoded with machine readable data which, when using a machine

programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a crystal structure according to any one of claims 1 to 17 or a homologue of said crystal structure.

19. A method for designing a potential glucocorticoid receptor ligand for the treatment of diseases modulated by the glucocorticoid, the method comprising the steps of:
- c) employing computational means to perform a fitting operation between the chemical entity and a binding site of GR receptors identified from a crystal according to any one of claims 1-17, or a 3D representation obtained from a machine-readable storage medium according to claim 18.
  - d) analyzing the results of the fitting operation to predict the association between the potential chemical entity and the binding site;
  - c) synthesizing the potential glucocorticoid receptor ligand based on the crystal structure of the glucocorticoid receptor;
  - e) assaying the glucocorticoid receptor ligand for glucocorticoid receptor binding, response in a glucocorticoid reporter cell line, measuring in vivo effects including but not limited to hepatic glucose production, marker proteins such as tyrosine amino transferase, corticotropin-releasing hormone, or antiinflammatory response which indicates that the compound may be used for treatment of diseases modulated by the glucocorticoid receptor.
20. A method according to claim 19, wherein the binding pocket resides in the ligand binding domain have been identified.
21. A method according to claim 19, wherein said potential glucocorticoid receptor ligand is a glucocorticoid receptor antagonist.

22. A method according to claim 19, wherein said potential glucocorticoid receptor ligand is an agonist.
23. A method of designing a ligand which will bind to GR comprising comparing the shape of a compound with the shape of the ligand binding domain of GR as obtained from a crystal according to any one of claims 1 to 17, and determining which amino acid or amino acids of the ligand binding domain interact with said compound.
24. A ligand identified by a method according to any one of claims 19 to 22.
25. A ligand according to claim 23 or claim 24 which is an agonist or antagonist of GR.
26. A crystallized molecule or molecular complex comprising a binding pocket defined by the structure coordinates of human GR ligand binding domain amino acid residues MET560, LEU563, ASN564, LEU566, GLY567, GLY568, GLN570, TRP600, MET601, MET604, ALA605, LEU608, PHE623, MET646, LEU732, CYS736, ALA748 or a homologue of said molecule or molecular complex wherein said homologue has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.
27. A machine-readable storage medium, comprising data storage material encoded with machine readable data, wherein the data is defined by all or a portion of the crystallized molecule or molecular complex according to claim 26.
28. A crystallisable composition comprising at least 150 amino acid residues of the GR ligand binding domain.
29. An isolated protein consisting of the amino acid sequence shown in Seq. ID1, Seq. ID2 or Seq. ID3.
30. An isolated protein having an amino acid sequence identical to the amino acid sequence used in a crystal according to any one of claims 1 to 6.

31. A method of obtaining structural information about a molecule or a molecular complex of unknown structure by using structure coordinates as set out for any one or more of the GR complexes shown in the Annex, comprising the steps of:

a) generating X-ray diffraction data from said crystallised molecule or molecular complex;

b) applying at least a portion of the structure coordinates set forth in the Annex to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex.

Affinity enhancing substituents marked by "R".

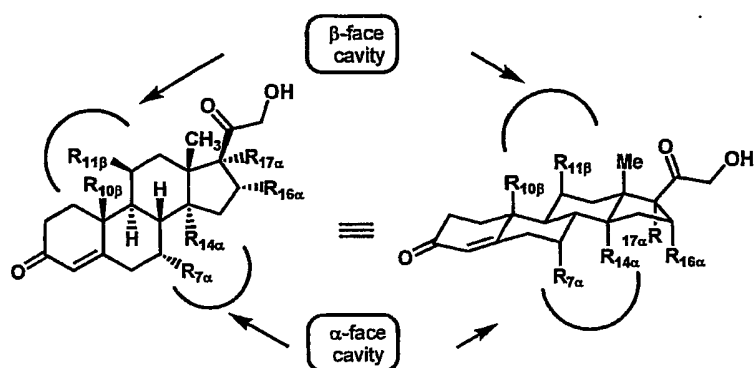
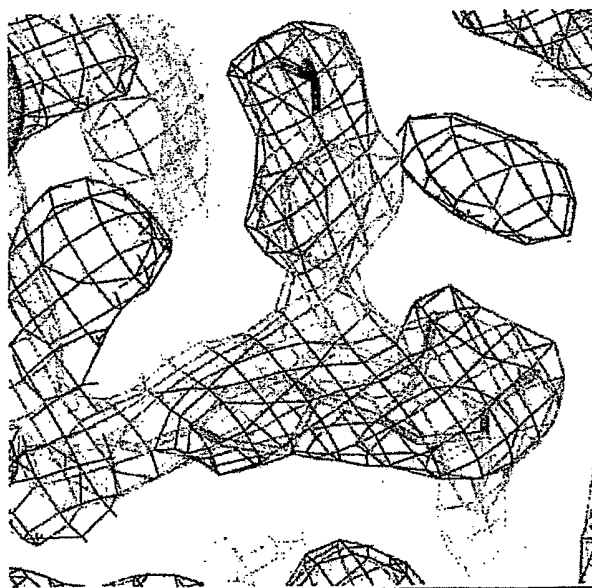


Figure 1.

Figure 2



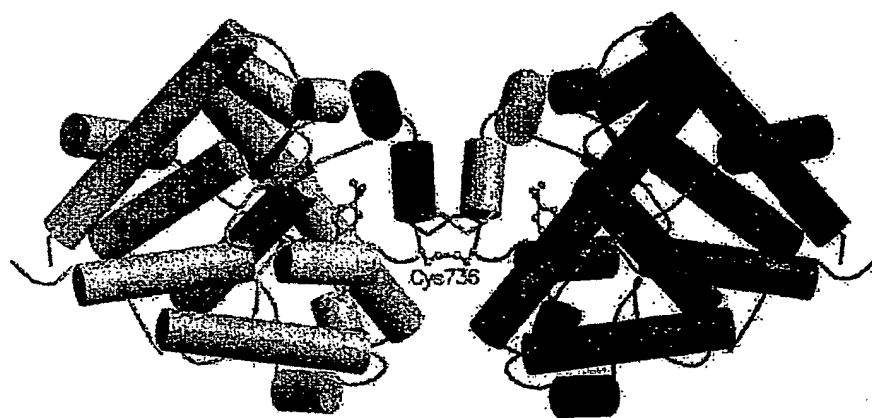


Figure 3

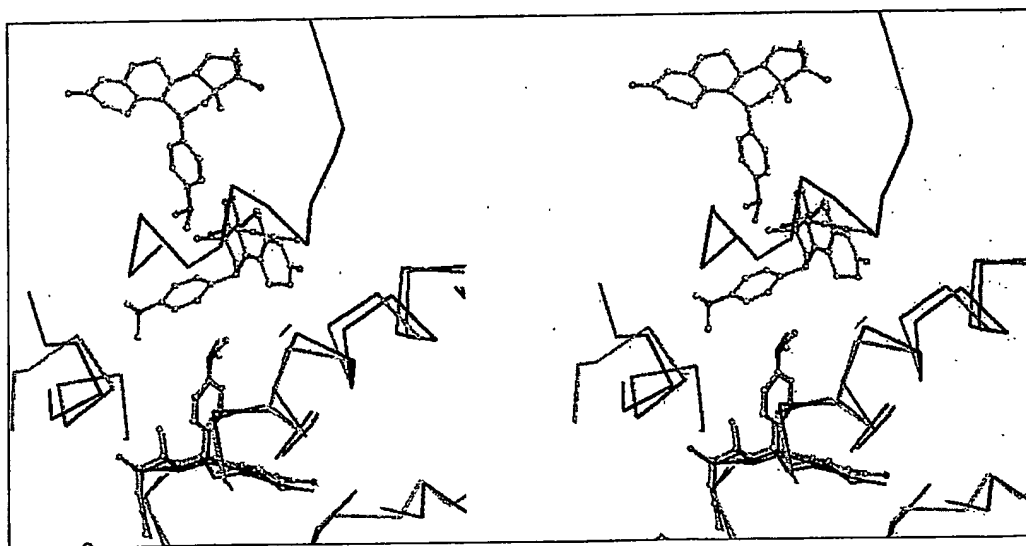


Figure 4

Figure 5

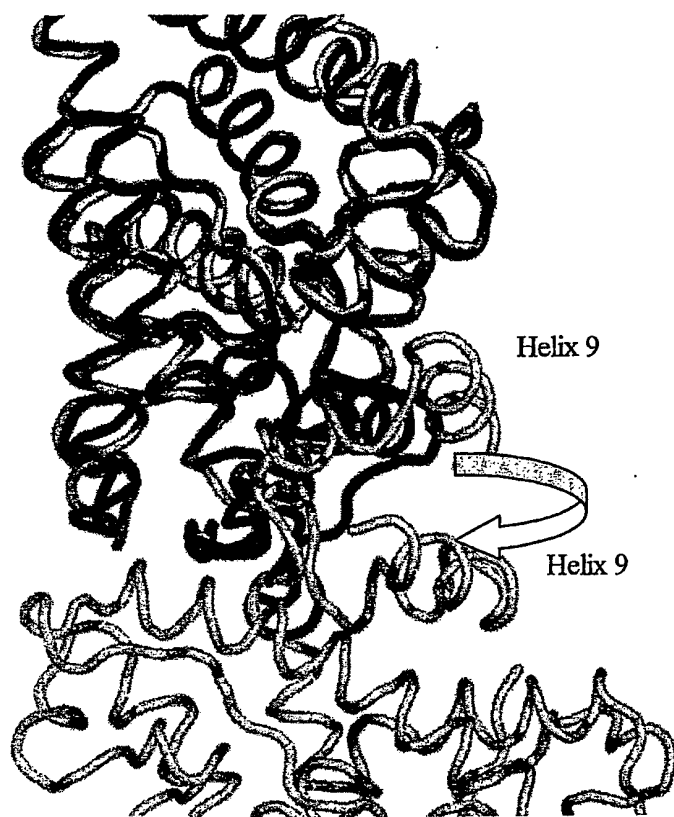


Figure 6

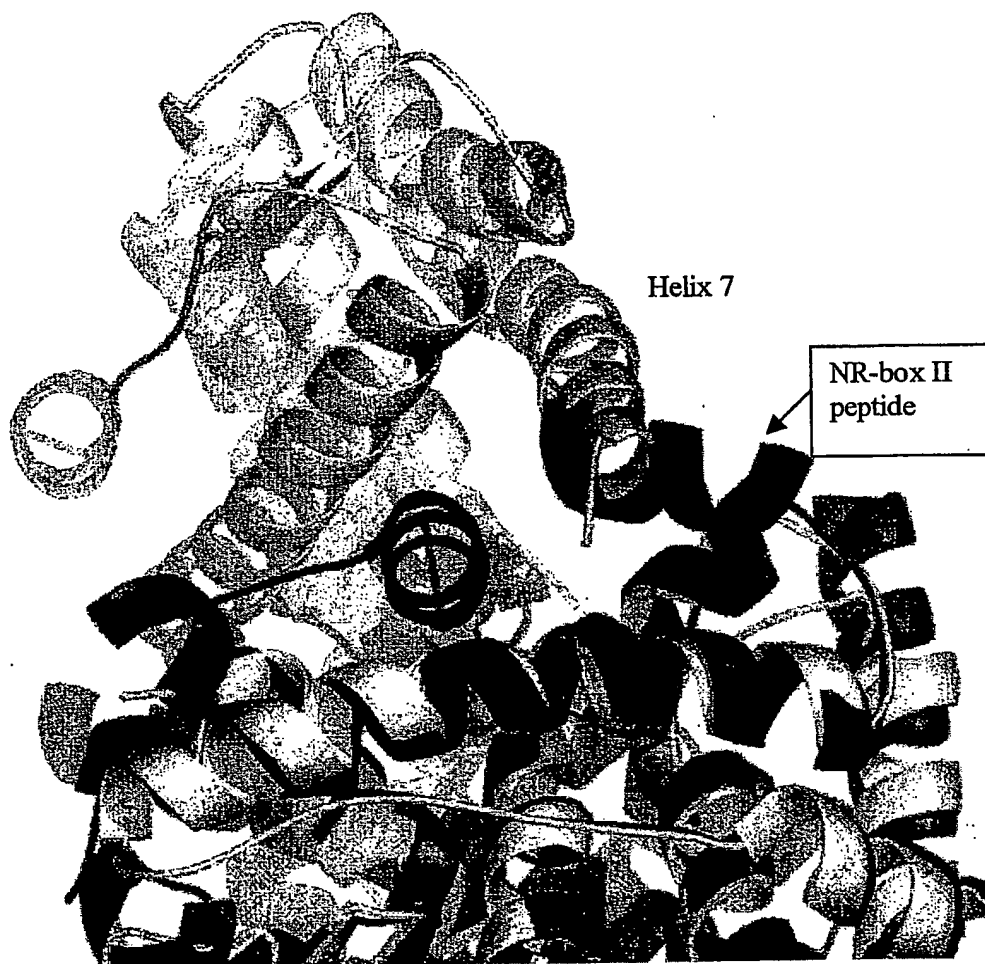


Figure 7

## CLUSTAL W (1.81) multiple sequence alignment

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GR3      -----
GR2      -----
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MDSKESLTPGREENPSSVLAQERGDVMDFYKTLRGGATVKVSASSPSLAV

GR1      -----
GR3      -----
GR2      -----
gi|121069|sp|P04150|GCR_HUMAN 100
ASQSDSKQRRLLVDFPKGSVSNAAQPDLSKAVSLSMGLYMGETETKVMGN

GR1      -----
GR3      -----
GR2      -----
gi|121069|sp|P04150|GCR_HUMAN 150
DLGFPOQGQISLSSGETDLKLEESIANLNRSTSVPENPKSSASTAVSAA

GR1      -----
GR3      -----
GR2      -----
gi|121069|sp|P04150|GCR_HUMAN 200
PTEKEFPKTHSDVSSEQQHLKGQTGTNGGNVKLYTTDQSTFDILQDLEFS

GR1      -----
GR3      -----
GR2      -----
gi|121069|sp|P04150|GCR_HUMAN 250
SGSPGKETNESPWRSDLLIDENCLLSPLAGEDDSFLEGNSEDCKPLIL
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6/8

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GR1 -----
GR3 -----
GR2 -----
gi|121069|sp|P04150|GCR_HUMAN 300
PDTKPKIKDNGDLVLSSPSNVTLPOVKTEKEDEFIELDCTPGVIKQEKLGTV

GR1 -----
GR3 -----
GR2 -----
gi|121069|sp|P04150|GCR_HUMAN 350
YQASFPGANLIGNKMSAISVHGVSSTSGGMYHYDMNTASLSQQQDQKPI

GR1 -----
GR3 -----
GR2 -----
gi|121069|sp|P04150|GCR_HUMAN 400
ENVIPPIPVGSENNRCQGGDDNLTSLGTLNFPGRVFSNGYSSPSMRP

GR1 -----
GR3 -----
GR2 -----
gi|121069|sp|P04150|GCR_HUMAN 450
DVSSPSSSSSTATTGPPPKICLVCSDEASGCHYGVLTCGCKVFFKRAVE

GR1 -----GSI 3
GR3 -----GSI 3
GR2 -----
gi|121069|sp|P04150|GCR_HUMAN 500
GQNYLCAGRNDCIIDKIRKNCPCACRYRKCLQAGMNLKARKTKKIKGI

GR1 -----
GR3 -----
GR2 -----
gi|121069|sp|P04150|GCR_HUMAN 53
QQATTGVSQETSENPNGKTIIVPATLPQLTPTIVSLLEVIEPEVLYAGYDS
QQATTGVSQETSENPNGKTIIVPATLPQLTPTIVSLLEVIEPEVLYAGYDS
-----TIVPATLPQLTPTIVSLLEVIEPEVLYAGYDS 32
QQATTGVSQETSENPNGKTIIVPATLPQLTPTIVSLLEVIEPEVLYAGYDS 550
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GR3 EMLAEIITNQIPKYSNGNIKKLLFHQK 280  
GR2 -----  
gi|121069|sp|P04150|GCR\_HUMAN EMLAEIITNQIPKYSNGNIKKLLFHQK 777  
H9

GR1  
GR3  
GR2  
gi|121069|sp|P04150|GCR\_HUMAN

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- (74) Agents: **ELSY, David et al.**; Withers & Rogers, Goldings House, 2 Hays Lane, London SE1 2HW (GB).
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(54) Title: GLUCOCORTICOID RECEPTOR PROTEIN CRYSTALS

(57) Abstract: The present invention is in the fields of biotechnology, protein purification and crystallization, x-ray diffraction analysis, three-dimensional computer molecular modeling and rational drug design. The invention is directed to the glucocorticoid receptor and ligands for this receptor, and in particular to crystalline glucocorticoid receptor (GR) and to methods of identifying ligands utilizing GR, as well as to compounds, compositions and methods for selecting, making, and using therapeutic or diagnostic agents having GR modulating or binding activity.



WO 2003/090666 A3

# INTERNATIONAL SEARCH REPORT

International Application No  
PCT/EP 03/04900

A. CLASSIFICATION OF SUBJECT MATTER  
IPC 7 C07K14/72 G06F19/00 G01N33/48

According to International Patent Classification (IPC) or to both national classification and IPC

## B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)  
IPC 7 C07K G06F G01N

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the International search (name of data base and, where practical, search terms used)

BIOSIS, EPO-Internal, WPI Data, PAJ, MEDLINE

## C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
P,X	WO 03 015692 A (APOLITO CHRISTOPHER J ;LAMBERT MILLARD H III (US); SMITHKLINE BEEC) 27 February 2003 (2003-02-27) the whole document ---	1-23, 26-31
P,X	RANDY K. BLEDSOE ET AL: "Crystal Structure of the Glucocorticoid Receptor Ligand Binding Domain Reveals a Novel Mode of Receptor Dimerization and Coactivator Recognition" CELL, vol. 110, 12 July 2002 (2002-07-12), pages 93-105, XP002257981 the whole document --- -/--	1-23, 26-31

☒ Further documents are listed in the continuation of box C.

☒ Patent family members are listed in annex.

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- "&" document member of the same patent family

Date of the actual completion of the international search

16 October 2003

Date of mailing of the international search report

07 NOV 2003

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## INTERNATIONAL SEARCH REPORT

International Application No

PCT/EP 03/04900

C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT		
Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
P,X	BRIAN M. NECELA ET AL: "Crystallization of the human glucocorticoid receptor ligand binding domain: a step towards selective glucocorticoids" TRENDS IN PHARMACOLOGICAL SCIENCES, vol. 24, no. 2, February 2003 (2003-02), pages 58-61, XP002257982 the whole document	1-23, 26-31
P,X	--- DATABASE MEDLINE [Online] US NATIONAL LIBRARY OF MEDICINE (NLM), BETHESDA, MD, US; 20 June 2003 (2003-06-20) KAUPPI BJÖRN ET AL: "The three-dimensional structures of antagonistic and agonistic forms of the glucocorticoid receptor ligand-binding domain: RU-486 induces a transconformation that leads to active antagonism." Database accession no. NLM12686538 XP002257983 abstract & THE JOURNAL OF BIOLOGICAL CHEMISTRY. UNITED STATES 20 JUN 2003, vol. 278, no. 25, 20 June 2003 (2003-06-20), pages 22748-22754, ISSN: 0021-9258	1-23, 26-31
X	--- DATABASE GENBANK ON NCBI [Online] Accession no. AAA16603; 10 March 1994 (1994-03-10) MUNROE, D. G. ET AL: "Alternative splicing within the DNA binding domain creates a novel isoform of the human glucocorticoid receptor" XP002257990 retrieved on 2003-10-10 abstract -& DATABASE GENBANK [Online] Accession no. AAA16603; XP002257991 Registry file RN 481222-48-4 99% identity in 276aa overlap with SEQ ID No 7, 99% identity in 224aa overlap with SEQ ID No 2, 98% identity in 275aa overlap with SEQ ID No 3 abstract --- -/--	29,30

## INTERNATIONAL SEARCH REPORT

International Application No

PCT/EP 03/04900

C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT		
Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	DATABASE REGISTRY FILE [Online] XP002258182 RN 289516-93-4 99% identity in 276aa with SEQ ID No 1 and 99% identity in 224aa with SEQ ID No 2, RN 289516-93-4 99% identity in 248aa with SEQ ID No 3 abstract	29,30
A	-& WO 00 52050 A (GILLNER M ET AL) 8 September 2000 (2000-09-08) figures 2A,11, ---	1-23, 26-28,31
A	CATHERINE ROBIN-JAGERSCHMIDT ET AL: "Residues in the Ligand Binding Domain That Confer Progestin or Glucocorticoid Specificity and Modulate the Receptor Transactivation Capacity" MOLECULAR ENDOCRINOLOGY, vol. 14, no. 7, 2000, pages 1028-1037, XP002257984	1-23, 26-28,31
X	the whole document ---	29,30
A	DATABASE MEDLINE [Online] US NATIONAL LIBRARY OF MEDICINE (NLM), BETHESDA, MD, US; August 2001 (2001-08) DEY R ET AL: "Homology modelling of the ligand-binding domain of glucocorticoid receptor: binding site interactions with cortisol and corticosterone." Database accession no. NLM11579225 XP002257985 abstract & PROTEIN ENGINEERING. ENGLAND AUG 2001, vol. 14, no. 8, August 2001 (2001-08), pages 565-571, ISSN: 0269-2139 ---	1-23, 26-31
A	WO 99 50658 A (GREENE GEOFFREY L ;AGARD DAVID A (US); ARCH DEV CORP (US); KUSHNER) 7 October 1999 (1999-10-07) the whole document ---	1-23, 26-31
A	B.F. LUISI ET AL: "Crystallographic analysis of the interaction of the glucocorticoid receptor with DNA" NATURE, vol. 352, 8 August 1991 (1991-08-08), pages 497-505, XP002257986 the whole document ---	1-23, 26-31
	---	
	-/--	

# INTERNATIONAL SEARCH REPORT

International Application No  
PCT/EP 03/04900

C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT		
Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	<p>WILLIAM BOURGUET ET AL: "Crystal structure of the ligand-binding domain of the human nuclear receptor RXR-alpha" NATURE, vol. 375, 1 June 1995 (1995-06-01), pages 377-382, XP002257987 the whole document</p>	1-23, 26-31
A	<p>YIHOUNG WAN ET AL: "Separable Features of the Ligand-Binding Domain Determine the Differential Subcellular Localization and Ligand-Binding Specificity of Glucocorticoid Receptor and Progesterone Receptor" MOLECULAR ENDOCRINOLOGY, vol. 15, no. 1, 2001, pages 17-31, XP002257988 the whole document</p>	1-23, 26-31
A	<p>DATABASE BIOSIS [Online] BIOSCIENCES INFORMATION SERVICE, PHILADELPHIA, PA, US; 23 June 2000 (2000-06-23) LIND ULRIKA ET AL: "Functional probing of the human glucocorticoid receptor steroid-interacting surface by site-directed mutagenesis: Gln-642 plays an important role in steroid recognition and binding" Database accession no. PREV200000369093 XP002257992 abstract &amp; JOURNAL OF BIOLOGICAL CHEMISTRY, vol. 275, no. 25, 23 June 2000 (2000-06-23), pages 19041-19049, ISSN: 0021-9258</p>	1-23, 26-31
A	<p>JAN- KE GUSTAFSSON ET AL: "Structure, function and regulation of the glucocorticoid receptor" PROGRESS IN CLINICAL AND BIOLOGICAL RESEARCH, vol. 322, 1990, pages 65-80, XP002257989 the whole document</p>	1-23, 26-31

## INTERNATIONAL SEARCH REPORT

International application No.  
PCT/EP 03/04900

### Box I Observations where certain claims were found unsearchable (Continuation of item 1 of first sheet)

This International Search Report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. ☐ Claims Nos.:  
because they relate to subject matter not required to be searched by this Authority, namely:
2. ☒ Claims Nos.: 24-25  
because they relate to parts of the International Application that do not comply with the prescribed requirements to such an extent that no meaningful International Search can be carried out, specifically:  
see FURTHER INFORMATION sheet PCT/ISA/210
3. ☐ Claims Nos.:  
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

### Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

1. ☐ As all required additional search fees were timely paid by the applicant, this International Search Report covers all searchable claims.
2. ☐ As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.
3. ☐ As only some of the required additional search fees were timely paid by the applicant, this International Search Report covers only those claims for which fees were paid, specifically claims Nos.:
4. ☐ No required additional search fees were timely paid by the applicant. Consequently, this International Search Report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

Remark on Protest

- ☐ The additional search fees were accompanied by the applicant's protest.
- ☐ No protest accompanied the payment of additional search fees.

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

Continuation of Box I.2

Claims Nos.: 24-25

Present claims 24-25 relate to compounds identified by the method disclosed in claims 19-22. Claims 24-25 relate to an extremely large number of possible compounds, including known compounds. Support within the meaning of Article 6 PCT and disclosure within the meaning of Article 5 is not to be found for any such compounds. In the present case, the claims so lack support and the application so lacks disclosure. These claims have not been searched.

The applicant's attention is drawn to the fact that claims, or parts of claims, relating to inventions in respect of which no international search report has been established need not be the subject of an international preliminary examination (Rule 66.1(e) PCT). The applicant is advised that the EPO policy when acting as an International Preliminary Examining Authority is normally not to carry out a preliminary examination on matter which has not been searched. This is the case irrespective of whether or not the claims are amended following receipt of the search report or during any Chapter II procedure.

# INTERNATIONAL SEARCH REPORT

Information on patent family members

International Application No

PCT/EP 03/04900

Patent document cited in search report		Publication date		Patent family member(s)		Publication date
WO 03015692	A	27-02-2003	WO	03015692 A2		27-02-2003
-----						
WO 0052050	A	08-09-2000	AU	2818200 A		21-09-2000
			WO	0052050 A2		08-09-2000
-----						
WO 9950658	A	07-10-1999	AU	3457199 A		18-10-1999
			AU	5769099 A		06-12-1999
			CA	2323575 A1		25-11-1999
			CA	2324060 A1		07-10-1999
			EP	1144997 A2		17-10-2001
			EP	1068529 A2		17-01-2001
			JP	2002516983 T		11-06-2002
			JP	2003523498 T		05-08-2003
			WO	9960014 A2		25-11-1999
			WO	9950658 A2		07-10-1999
			US	2002061539 A1		23-05-2002
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